2.3 Feldoperatoren

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

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

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

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

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

Teilchenzahlop. $\hat{N} = \sum_{\nu=1}^{\infty} a_\nu^+ a_\nu = \int \hat{\psi}^+(\underline{x})\, \hat{\psi}(\underline{x})\, d\tau$

Einteilchenenergieoperator

$$\hat{H} = \sum_{\lambda,\mu}^{1\ldots\infty} A_{\lambda\mu}\, a_\lambda^+ a_\mu = \int \hat{\psi}^+(\underline{x})\, A(\underline{x})\, \hat{\psi}(\underline{x})\, d\tau$$

2.4 Elektronengas

A Spinoren in Schrödinger-Darstellung

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

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

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

B Feldoperatoren als Spinoren

$\varphi_\nu(\vec{r})$ sei eine Basis in $\mathcal{H}_o$

$$\hat{\psi}_\sigma(\vec{r}) = \sum_{\nu=1}^{\infty} \varphi_\nu(\vec{r})\, a_{\nu\sigma} \quad ; \quad a_{\nu\sigma} = \int \varphi_\nu^*(\vec{r})\, \hat{\psi}_\sigma(\vec{r})\, d^3r \qquad \Big|\ \sigma = \pm\tfrac{1}{2}$$

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

Antivertauschungsrelationen

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

Teilchenzahloperator

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

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

Teilchendichteoperator

C Energieoperator

Potenzialoperator

$$H\Psi_g(\vec r_1 \ldots \vec r_N) = E_g \Psi_g(\vec r_1 \ldots \vec r_N)$$

N-Elektronen-Schrödinger-Glg. $\quad \langle \Psi_g | \Psi_g \rangle = 1$

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

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

$$\boxed{V} \cong \langle \Psi^{SD} | \sum_{i=1}^{N} v(\vec r_i) | \Psi^{SD} \rangle$$

Thomas, Fermi

$$= \sum_{i=1}^{N} \int \varphi^*_{k_i}(\vec r_i)\, v(\vec r_i)\, \varphi_{k_i}(\vec r_i)\, d^3r_i$$

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

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

$$\hat V = \int \hat n(\vec r)\, v(\vec r)\, d^3r$$

$$V = \langle \Psi_g | \hat V | \Psi_g \rangle$$
$$= \int \langle \Psi_g | \hat n(\vec r)\, v(\vec r) | \Psi_g \rangle\, d^3r$$
$$= \int \langle \Psi_g | \hat n(\vec r) | \Psi_g \rangle\, v(\vec r)\, d^3r$$
$$= \int n_g(\vec r)\, v(\vec r)\, d^3r \quad \vdots$$