I. ONE ELECTRON

quantum state: $|\psi\rangle$.

Wave function: $\psi(\mathbf{x}) \equiv \langle \mathbf{x}|\psi\rangle$ in the ortho-normal complete basis $\{|\mathbf{x}\rangle\}$ (eigenstates of the position operator) obeying

$$\int d\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}| = 1,$$

$$\langle \mathbf{x}|\mathbf{x}'\rangle = \delta(\mathbf{x}-\mathbf{x}'),$$

Normalization:

$$1 = \langle\psi|\psi\rangle = \langle\psi| \left(\int d\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|\right) |\psi\rangle = \int d\mathbf{x}\, \psi^*(\mathbf{x})\psi(\mathbf{x}) = \int d\mathbf{x}\, |\psi(\mathbf{x})|^2 .$$

Under any ortho-normal complete basis $\{|n\rangle\}$ obeying

$$\sum_n |n\rangle\langle n| = 1,$$

$$\langle n|n'\rangle = \delta_{n,n'},$$

we define $\psi_n \equiv \langle n|\psi\rangle$, then the normalization:

$$1 = \langle\psi|\psi\rangle = \langle\psi| \left(\sum_n |n\rangle\langle n|\right) |\psi\rangle = \sum_n \langle\psi|n\rangle\langle n|\psi\rangle = \sum_n |\psi_n|^2.$$

Position operator $\hat{\mathbf{r}}$:

$$\mathbf{r}|\mathbf{x}\rangle = \mathbf{x}|\mathbf{x}\rangle,$$

$$\langle\mathbf{x}|\hat{\mathbf{r}} = \langle\mathbf{x}|\mathbf{x}.$$

Momentum operator $\hat{\mathbf{p}}$. All eigenstates of $\hat{\mathbf{p}}$ form an ortho-normal complete basis $\{|\mathbf{k}\rangle\}$:

$$\sum_{\mathbf{k}} |\mathbf{k}\rangle\langle\mathbf{k}| = 1,$$

$$\langle\mathbf{k}|\mathbf{k}'\rangle = \delta_{\mathbf{k},\mathbf{k}'},$$

Box normalization inside a box with volumne V. Normalized eigenstate:

$$\langle\mathbf{x}|\mathbf{k}\rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{x}}.$$

$$\langle\mathbf{k}|\mathbf{k}\rangle = \langle\mathbf{k}| \left(\int d\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|\right) \mathbf{k}\rangle = \int d\mathbf{x}\, |\langle\mathbf{x}|\mathbf{k}\rangle|^2 = \int d\mathbf{x}\, \frac{1}{V} = 1.$$

Particle number operator: $\hat{N} = 1$. Particle density operator: $\hat{N}(\mathbf{x}) = \hat{N}\delta(\hat{\mathbf{r}} - \mathbf{x}) = \delta(\hat{\mathbf{r}} - \mathbf{x})$.

$$\int d\mathbf{x}\, \hat{N}(\mathbf{x}) = \hat{N} = 1.$$

Position operator $\hat{\mathbf{r}}$. Position density operator: $\hat{\mathbf{r}}(\mathbf{x}) = \hat{\mathbf{r}}\delta(\hat{\mathbf{r}} - \mathbf{x}) = \delta(\hat{\mathbf{r}} - \mathbf{x})\hat{\mathbf{r}} = \mathbf{x}\delta(\hat{\mathbf{r}} - \mathbf{x})$.

$$\int d\mathbf{x}\, \hat{\mathbf{r}}(\mathbf{x}) = \hat{\mathbf{r}}.$$

Momentum operator $\hat{\mathbf{p}}$. Momentum density operator

$$\hat{\mathbf{p}}(\mathbf{x}) \equiv \frac{\delta(\hat{\mathbf{r}} - \mathbf{x})\hat{\mathbf{p}} + \hat{\mathbf{p}}\delta(\hat{\mathbf{r}} - \mathbf{x})}{2} \Rightarrow \int d\mathbf{x}\, \hat{\mathbf{p}}(\mathbf{x}) = \hat{\mathbf{p}}.$$

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Given the quantum state $\psi(\mathbf{x}) = \langle \mathbf{x}|\psi\rangle$ of the particle.

The average particle number is

$$\langle\psi|\hat{N}|\psi\rangle = \langle\psi|\psi\rangle = 1.$$

The average particle density at $\mathbf{x}$ is

$$\langle\psi|\hat{N}(\mathbf{x})|\psi\rangle = \int d\mathbf{x}'\, \langle\psi|\delta(\hat{\mathbf{r}} - \mathbf{x})\,|\mathbf{x}'\rangle\langle\mathbf{x}'|\psi\rangle = \int d\mathbf{x}'\, \langle\psi|\delta(\mathbf{x}' - \mathbf{x})\,|\mathbf{x}'\rangle\langle\mathbf{x}'|\psi\rangle = |\psi(\mathbf{x})|^2 .$$

The average position is

$$\langle\psi|\hat{\mathbf{r}}|\psi\rangle = \langle\psi|\hat{\mathbf{r}} \int d\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|\psi\rangle = \int \mathbf{x} d\mathbf{x}\, \langle\psi|\mathbf{x}\rangle\langle\mathbf{x}|\psi\rangle = \int \mathbf{x}\, |\psi(\mathbf{x})|^2\, d\mathbf{x}.$$

The average momentum is

$$\langle\psi|\hat{\mathbf{p}}|\psi\rangle = \langle\psi| \int d\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|\hat{\mathbf{p}}|\psi\rangle = \int d\mathbf{x}\, \psi^*(\mathbf{x})\langle\mathbf{x}|\hat{\mathbf{p}}|\psi\rangle = \int d\mathbf{x}\, \psi^*(\mathbf{x})\left[-i\nabla_{\mathbf{x}}\psi(\mathbf{x})\right].$$

The average momentum density is

$$\begin{aligned}
\langle\psi|\hat{\mathbf{p}}(\mathbf{x})|\psi\rangle &= \langle\psi|\frac{\delta(\hat{\mathbf{r}} - \mathbf{x})\hat{\mathbf{p}} + \hat{\mathbf{p}}\delta(\hat{\mathbf{r}} - \mathbf{x})}{2}|\psi\rangle = \langle\psi| \int d\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}|\frac{\delta(\hat{\mathbf{r}} - \mathbf{x})\hat{\mathbf{p}} + \hat{\mathbf{p}}\delta(\hat{\mathbf{r}} - \mathbf{x})}{2}|\psi\rangle \\
&= \frac{1}{2}\langle\psi| \int d\mathbf{x}'\, |\mathbf{x}'\rangle\langle\mathbf{x}'|\delta(\hat{\mathbf{r}} - \mathbf{x})\hat{\mathbf{p}}|\psi\rangle + \frac{1}{2}\langle\psi| \int d\mathbf{x}'\, |\mathbf{x}'\rangle\langle\mathbf{x}'|\hat{\mathbf{p}}\delta(\hat{\mathbf{r}} - \mathbf{x})|\psi\rangle \\
&= \frac{1}{2}\int \delta(\mathbf{x}' - \mathbf{x})d\mathbf{x}'\, \langle\psi|\mathbf{x}'\rangle(-i\nabla_{\mathbf{x}'})\langle\mathbf{x}'|\psi\rangle + \frac{1}{2}\int d\mathbf{x}'\, \langle\psi|\mathbf{x}'\rangle(-i\nabla_{\mathbf{x}'})\left[\delta(\mathbf{x}' - \mathbf{x})\langle\mathbf{x}'|\psi\rangle\right] \\
&= \frac{1}{2}\int \delta(\mathbf{x}' - \mathbf{x})d\mathbf{x}'\, \psi^*(\mathbf{x}')[-i\nabla_{\mathbf{x}'}\psi(\mathbf{x}')] + \frac{1}{2}\int d\mathbf{x}'\, \langle\psi|\mathbf{x}'\rangle(-i\nabla_{\mathbf{x}'})\left[\delta(\mathbf{x}' - \mathbf{x})\langle\mathbf{x}'|\psi\rangle\right] \\
&= \frac{1}{2}\psi^*(\mathbf{x})[-i\nabla_{\mathbf{x}}\psi(\mathbf{x})] + \frac{1}{2}\int d\mathbf{x}'\, \psi^*(\mathbf{x}')(-i\nabla_{\mathbf{x}'})\left[\delta(\mathbf{x}' - \mathbf{x})\psi(\mathbf{x}')\right].
\end{aligned}$$

The second term is (trick 1):

$$\begin{aligned}
\frac{1}{2}\int d\mathbf{x}'\,\psi^*(\mathbf{x}')(-i\nabla_{\mathbf{x}'})\left[\delta(\mathbf{x}'-\mathbf{x})\psi(\mathbf{x}')\right] &= \frac{1}{2}\int d\mathbf{x}'\,\psi^*(\mathbf{x}')\psi(\mathbf{x})(-i\nabla_{\mathbf{x}'})\delta(\mathbf{x}'-\mathbf{x}) \\
&= \frac{1}{2}\int d\mathbf{x}'\,\psi^*(\mathbf{x}')\psi(\mathbf{x})(i\nabla_{\mathbf{x}})\delta(\mathbf{x}'-\mathbf{x}) \\
&= \frac{1}{2}\psi(\mathbf{x})(i\nabla_{\mathbf{x}})\int d\mathbf{x}'\,\psi^*(\mathbf{x}')\delta(\mathbf{x}'-\mathbf{x}) \\
&= \frac{1}{2}\psi(\mathbf{x})(i\nabla_{\mathbf{x}})\psi^*(\mathbf{x}).
\end{aligned}$$

(integration by parts):

$$\begin{aligned}
\frac{-i}{2}\int d\mathbf{x}'\,\psi^*(\mathbf{x}')\nabla_{\mathbf{x}'}\left[\delta(\mathbf{x}'-\mathbf{x})\psi(\mathbf{x}')\right] &= \frac{-i}{2}\,\psi^*(\mathbf{x}')\left[\delta(\mathbf{x}'-\mathbf{x})\psi(\mathbf{x}')\right]|_{\mathbf{x}'=boundary} \\
&\quad - \frac{-i}{2}\int d\mathbf{x}'\,\left[\nabla_{\mathbf{x}'}\psi^*(\mathbf{x}')\right]\delta(\mathbf{x}'-\mathbf{x})\psi(\mathbf{x}') \\
&= \frac{i}{2}\left[\nabla_{\mathbf{x}}\psi^*(\mathbf{x})\right]\psi(\mathbf{x})
\end{aligned}$$

Finally, we have

$$\langle\psi|\hat{\mathbf{p}}(\mathbf{x})|\psi\rangle = \langle\psi|\frac{\delta(\hat{\mathbf{r}}-\mathbf{x})\hat{\mathbf{p}}+\hat{\mathbf{p}}\delta(\hat{\mathbf{r}}-\mathbf{x})}{2}|\psi\rangle = \frac{1}{2}\psi^*(\mathbf{x})(-i\nabla_{\mathbf{x}})\psi(\mathbf{x}) + \frac{1}{2}\left[(i\nabla_{\mathbf{x}})\psi^*(\mathbf{x})\right]\psi(\mathbf{x}).$$

Particle current operator:

$$\hat{\mathbf{J}} = \frac{\hat{\mathbf{p}}}{m_0}.$$

Particle current density operator at $\mathbf{x}$:

$$\hat{\mathbf{J}}(\mathbf{x}) = \frac{\delta(\hat{\mathbf{r}}-\mathbf{x})\hat{\mathbf{p}}+\hat{\mathbf{p}}\delta(\hat{\mathbf{r}}-\mathbf{x})}{m_0} = \frac{\hat{\mathbf{p}}(\mathbf{x})}{m_0}.$$

$$\begin{aligned}
\langle\psi|\hat{\mathbf{J}}(\mathbf{x})|\psi\rangle &= \frac{1}{2m_0}\psi^*(\mathbf{x})(-i\nabla_{\mathbf{x}})\psi(\mathbf{x}) + \frac{1}{2m_0}\left[(i\nabla_{\mathbf{x}})\psi^*(\mathbf{x})\right]\psi(\mathbf{x}) \\
&= \frac{-i}{2m_0}\left[\psi^*(\nabla_{\mathbf{x}}\psi)-(\nabla_{\mathbf{x}}\psi^*)\psi\right].
\end{aligned}$$

****************IMPORTANT ****************

$$\langle\mathbf{x}|\hat{\mathbf{p}}|\psi\rangle = \langle\mathbf{x}|\sum_{\mathbf{k}}|\mathbf{k}\rangle\langle\mathbf{k}|\hat{\mathbf{p}}|\psi\rangle = \sum_{\mathbf{k}}\mathbf{k}\langle\mathbf{x}|\mathbf{k}\rangle\langle\mathbf{k}|\psi\rangle = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}}\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{x}}\langle\mathbf{k}|\psi\rangle$$

$$i\nabla_{\mathbf{x}}\langle\mathbf{x}|\psi\rangle = \sum_{\mathbf{k}}i\nabla_{\mathbf{x}}\langle\mathbf{x}|\mathbf{k}\rangle\langle\mathbf{k}|\psi\rangle = -\sum_{\mathbf{k}}\frac{1}{\sqrt{V}}\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{x}}\langle\mathbf{k}|\psi\rangle,$$

thus

$$\langle\mathbf{x}|\hat{\mathbf{p}}|\psi\rangle = -i\nabla_{\mathbf{x}}\langle\mathbf{x}|\psi\rangle = -i\nabla_{\mathbf{x}}\psi(\mathbf{x}).$$

$$\langle\mathbf{x}|\hat{\mathbf{p}}\cdots = -i\nabla_{\mathbf{x}}\langle\mathbf{x}|\cdots$$

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II. MANY PARTICLES (NON-INTERACTING)

The Hamiltonian of a single electron is $\hat{H} = \hat{p}^2/(2m_0) + V(\hat{\mathbf{r}})$.

Many-body Hamiltonian $\hat{\mathcal{H}} = \sum_i \hat{H}_i,\ \hat{H}_i = \hat{p}_i^2/(2m_0) + V(\hat{\mathbf{r}}_i)$.

It suffices to treat the single-particle problem ******************

$$\hat{H}|\psi_k\rangle = E_k|\psi_k\rangle,$$
$$\hat{H}^n|\psi_k\rangle = E_k^n|\psi_k\rangle,$$
$$g(\hat{H}) = g(E_k)|\psi_k\rangle.$$

$$\sum_k |\psi_k\rangle\langle\psi_k| = 1,\ \langle\psi_k|\psi_{k'}\rangle = \delta_{kk'}.$$

Single-electron Green's function

$$\hat{G}(E) = \frac{1}{E - \hat{H} + i0^+},$$

$$G(E, \mathbf{x}_1, \mathbf{x}_2) = \langle\mathbf{x}_1|\frac{1}{E - \hat{H} + i0^+}|\mathbf{x}_2\rangle = \sum_k \langle\mathbf{x}_1|\frac{1}{E - E_k + i0^+}|\psi_k\rangle\psi_k^*(\mathbf{x}_2) = \sum_k \frac{\psi_k(\mathbf{x}_1)\psi_k^*(\mathbf{x}_2)}{E - E_k + i0^+}.$$

Local density of states:

$$\rho(E, \mathbf{x}) = -\frac{1}{\pi}\,\mathrm{Im}\,G(E, \mathbf{x}, \mathbf{x}) = -\frac{1}{\pi}\sum_k |\psi_k(\mathbf{x})|^2\,\mathrm{Im}\,\frac{1}{E - E_k + i0^+} = \sum_k |\psi_k(\mathbf{x})|^2\,\delta(E - E_k).$$

upon using $1/(x + i0^+) = P(1/x) - \pi i\delta(x)$.

Density of states:

$$\rho(E) \equiv \sum_k \delta(E - E_k).$$

************* Many particles ************

Given the Fermi energy E_F, the Fermi distribution is $f(E) = \frac{1}{e^{\beta(E-E_F)}+1}$, $\beta = 1/(k_B T)$.

With $O(\mathbf{x})$ for the single-particle operator and

$$\mathcal{O}(\mathbf{x}) = \sum_{i=1}^{N} O_i(\mathbf{x}) = \sum_{k,k'} \langle\psi_k|O(\mathbf{x})|\psi_{k'}\rangle\, C_k^\dagger C_{k'}$$

for the many-particle operator, where $C_k^\dagger$ creates a particle in the eigenstate $|\psi_k\rangle$, e.g., $C_k^\dagger|0\rangle = |1_k\rangle$, we have

$$\begin{aligned}\langle \mathcal{O}(\mathbf{x})\rangle &= \sum_{k,k'} \langle \psi_k|O(\mathbf{x})|\psi_{k'}\rangle \left\langle C_k^\dagger C_{k'}\right\rangle \\ &= \sum_{k,k'} \langle \psi_k|O(\mathbf{x})|\psi_{k'}\rangle\, \delta_{k,k'} f(E_k) \\ &= \sum_{k} \langle \psi_k|O(\mathbf{x})|\psi_{k}\rangle\, f(E_k).\end{aligned}$$

The total number of electrons is

$$\mathcal{N} = \sum_k \left\langle \psi_k|\hat{N}|\psi_k\right\rangle f(E_k) = \sum_k f(E_k) = \int dE \sum_k f(E_k)\delta(E-E_k) = \int f(E)\rho(E)dE$$

Electron density at $\mathbf{x}$:

$$\mathcal{N}(\mathbf{x}) \equiv \left\langle \hat{\mathcal{N}}(\mathbf{x})\right\rangle = \sum_k \left\langle \psi_k|\hat{N}(\mathbf{x})|\psi_k\right\rangle f(E_k) = \sum_k |\psi_k(\mathbf{x})|^2 f(E_k) = \int f(E)\rho(E,\mathbf{x})dE.$$

$$\rho(E,\mathbf{x}) = -\frac{1}{\pi}\operatorname{Im} G(E,\mathbf{x},\mathbf{x}) = \sum_k |\psi_k(\mathbf{x})|^2\, \delta(E-E_k).$$

$$\int d\mathbf{x}\, \rho(E,\mathbf{x}) = \rho(E).$$

$$\begin{aligned}\delta\rho(\mathbf{x},E) &= \rho(\mathbf{x},E) - \rho_0(\mathbf{x},E) \\ &= -\frac{1}{\pi}\operatorname{Im} G(E,\mathbf{x},\mathbf{x}) - \left[-\frac{1}{\pi}\operatorname{Im} G_0(E,\mathbf{x},\mathbf{x})\right]\end{aligned}$$

$$\begin{aligned}\hat{G}(E) &= \frac{1}{E-\hat{H}+i0^+}, \\ \hat{G}_0(E) &= \frac{1}{E-\hat{H}_0+i0^+}.\end{aligned}$$

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