THE POSITION OPERATOR

What is $\langle \psi_i | \mathbf{r} | \psi_f \rangle$?

Consider:
$$\langle \psi_i | \mathbf{p} | \psi_f \rangle = \langle \psi_i | [H, \mathbf{r}] | \psi_f \rangle = \langle \psi_i | H \mathbf{r} | \psi_f \rangle - \langle \psi_i | \mathbf{r} H | \psi_f \rangle = (\varepsilon_i - \varepsilon_f) \langle \psi_i | \mathbf{r} | \psi_f \rangle$$

And so:
$$\langle \psi_i | \mathbf{r} | \psi_f \rangle = \langle \psi_i | \mathbf{p} | \psi_f \rangle / (\varepsilon_i - \varepsilon_f)$$

NORM CONSERVING PSEUDOPOTENTIALS

What is $\langle\psi_i|\mathbf{r}|\psi_f\rangle$ for a non local pseudopotential?

Consider:
$$\langle\psi_i|\mathbf{p}|\psi_f\rangle + \langle\psi_i|[V_{\mathrm{nl}},\mathbf{r}]|\psi_f\rangle = \langle\psi_i|[H,\mathbf{r}]|\psi_f\rangle = \langle\psi_i|H\mathbf{r}|\psi_f\rangle - \langle\psi_i|\mathbf{r}H|\psi_f\rangle = (\varepsilon_i - \varepsilon_f)\langle\psi_i|\mathbf{r}|\psi_f\rangle$$

And so:
$$\langle\psi_i|\mathbf{r}|\psi_f\rangle = (\langle\psi_i|\mathbf{p}|\psi_f\rangle + \langle\psi_i|[V_{\mathrm{nl}},\mathbf{r}]|\psi_f\rangle)/(\varepsilon_i - \varepsilon_f)$$

Ultrasoft Pseudopotentials

What is $\langle \psi_i | \mathbf{r} | \psi_f \rangle$ when $H\Psi = ES\Psi$?

Consider:
$$\langle \psi_i | \mathbf{p} | \psi_f \rangle + \langle \psi_i | [V_{\mathrm{nl}}, \mathbf{r}] | \psi_f \rangle = \langle \psi_i | [H, \mathbf{r}] | \psi_f \rangle = \langle \psi_i | H\mathbf{r} | \psi_f \rangle - \langle \psi_i | \mathbf{r}H | \psi_f \rangle =$$
$$(\varepsilon_i - \varepsilon_f)\langle \psi_i | \mathbf{r} | \psi_f \rangle + \varepsilon_i \langle \psi_i | \Delta S \mathbf{r} | \psi_f \rangle - \varepsilon_f \langle \psi_i | \mathbf{r} \Delta S | \psi_f \rangle$$

And so:
$$\langle \psi_i | \mathbf{r} | \psi_f \rangle =$$
$$(\langle \psi_i | \mathbf{p} | \psi_f \rangle + \langle \psi_i | [V_{\mathrm{nl}}, \mathbf{r}] | \psi_f \rangle - \varepsilon_i \langle \psi_i | \Delta S \mathbf{r} | \psi_f \rangle + \varepsilon_f \langle \psi_i | \mathbf{r} \Delta S | \psi_f \rangle)/(\varepsilon_i - \varepsilon_f)$$

DIELECTRIC FUNCTION OF ZnS