density-functional perturbation theory

forces, response functions, phonons, and all that

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response functions

$$\text{property} = \frac{\partial(\text{variable})}{\partial(\text{strength})}$$

response functions

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- polarizability, dielectric constant $\dfrac{\partial \mathrm{P}_i}{\partial \mathrm{E}_j}$
- elastic constants $\dfrac{\partial \sigma_{ij}}{\partial \epsilon_{kl}}$
- piezoelectric constants $\dfrac{\partial \mathrm{P}_i}{\partial \epsilon_{kl}}$
- interatomic force constants $\dfrac{\partial f_i^s}{\partial u_j^t}$
- Born effective charges $\dfrac{\partial d_i^s}{\partial u_j^s}$
- ... $\cdots$

susceptibilities from perturbation theory

$$\hat{H}_\alpha = \hat{H}^\circ + \alpha \hat{A}$$

$$\chi_{BA} = \frac{\partial \langle \hat{B} \rangle_\alpha}{\partial \alpha}$$

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$$\langle \hat{B} \rangle = \frac{\partial E_\beta}{\partial \beta}$$

$$\hat{H}_\beta = \hat{H}^\circ + \beta \hat{B}$$ (Hellmann & Feynman)

susceptibilities from perturbation theory

$$\hat{H}_\alpha = \hat{H}^\circ + \alpha\hat{A}$$

$$\chi_{BA} = \frac{\partial\langle\hat{B}\rangle_\alpha}{\partial\alpha}$$

$$\langle\hat{B}\rangle = \frac{\partial E_\beta}{\partial\beta}$$

$$\hat{H}_\beta = \hat{H}^\circ + \beta\hat{B}$$

(Hellmann & Feynman)

$$\hat{H}_{\alpha\beta} = \hat{H}^\circ + \alpha\hat{A} + \beta\hat{B}$$

$$\boxed{\chi_{BA} = \frac{\partial^2 E_{\alpha\beta}}{\partial\alpha\partial\beta}}$$

energy derivatives

$$H = H_0 + \sum_i \lambda_i v_i$$

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$$E[\lambda] = E_0 - \sum_i f_i \lambda_i + \frac{1}{2} \sum_{ij} h_{ij} \lambda_i \lambda_j + \cdots$$

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- structural optimization & molecular dynamics

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- structural optimization & molecular dynamics
- (static) response functions

  elastic constants

  dielectric tensor

  piezoelectric tensor

  Born effective charges

  . . .

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- structural optimization & molecular dynamics
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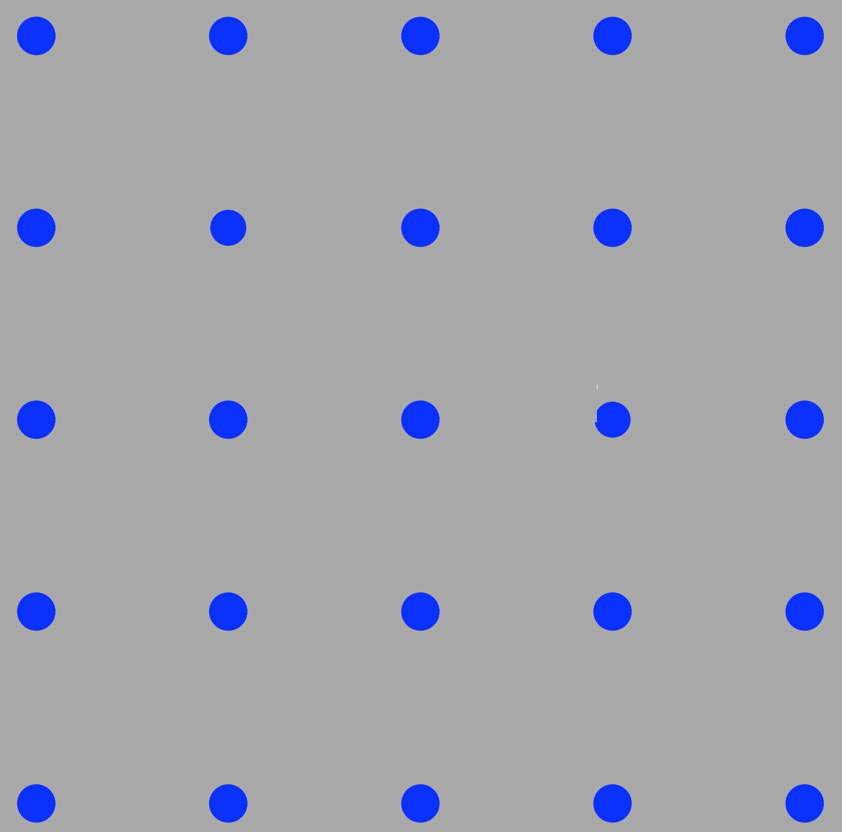
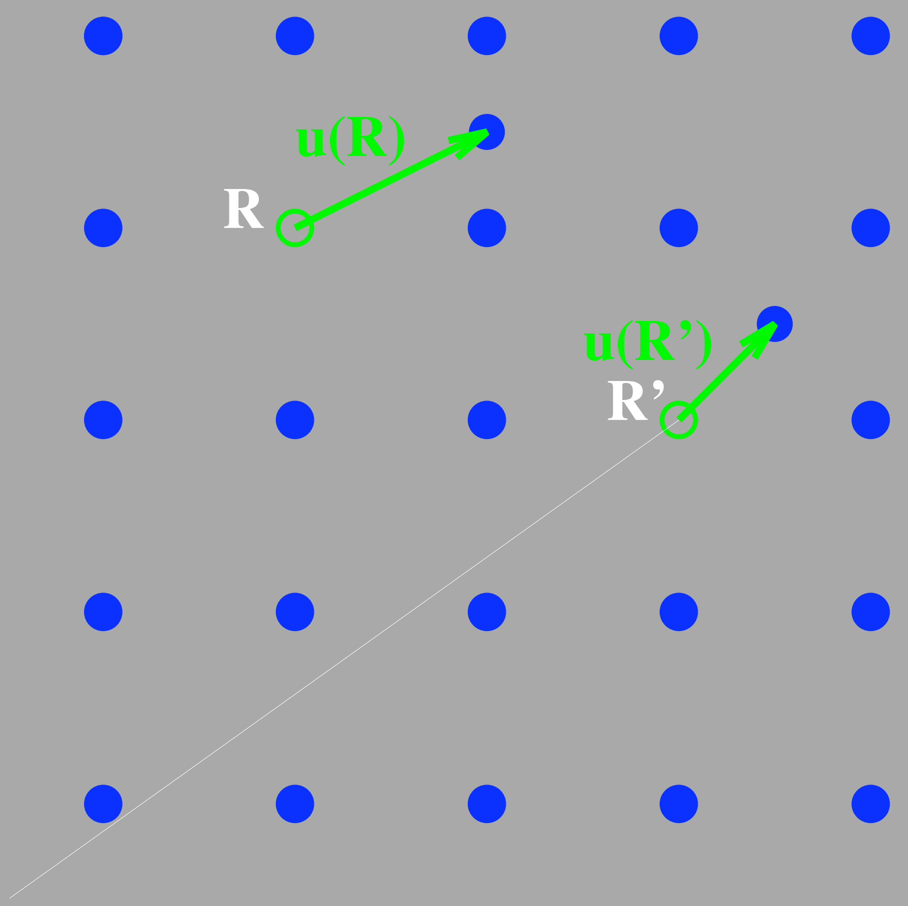
  . . .
- vibrational modes in the adiabatic approximaton

lattice dynamics



$$
\begin{aligned}
V(\mathbf{r}) &= V_0(\mathbf{r}) \\
&= \sum_{\mathbf{R}} v(\mathbf{r} - \mathbf{R}) \\
E &= E_0
\end{aligned}
$$

lattice dynamics



$$
\begin{aligned}
V(\mathbf{r}) &= V_0(\mathbf{r}) \\
&\quad + \sum_{\mathbf{R}} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial v(\mathbf{r}-\mathbf{R})}{\partial \mathbf{R}}
\end{aligned}
$$

$$
\begin{aligned}
E &= E_0 \\
&\quad + \frac{1}{2} \sum_{\mathbf{R},\mathbf{R}'} \mathbf{u}(\mathbf{R}) \cdot \frac{\partial^2 E}{\partial \mathbf{u}(\mathbf{R}) \partial \mathbf{u}(\mathbf{R}')} \cdot \mathbf{u}(\mathbf{R}') \\
&\quad + \cdots
\end{aligned}
$$

energy derivatives and perturbation theory

$$H = H_0 + \sum_i \lambda_i v_i \qquad E[\lambda] = E_0 - \sum_i f_i \lambda_i + \frac{1}{2} \sum_{ij} h_{ij} \lambda_i \lambda_j + \cdots$$

energy derivatives and perturbation theory

$$H = H_0 + \sum_i \lambda_i v_i \qquad\qquad E[\lambda] = E_0 - \sum_i f_i \lambda_i + \frac{1}{2}\sum_{ij} h_{ij}\lambda_i\lambda_j + \cdots$$

$$f_i = -\left.\frac{\partial E}{\partial \lambda_i}\right|_{\lambda=0} \quad = \quad -\langle \Psi_0 | v_i | \Psi_0 \rangle$$

energy derivatives and perturbation theory

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$$h_{ij} = \left. \frac{\partial^2 E}{\partial \lambda_i \partial \lambda_j} \right|_{\lambda=0} = 2 \sum_n \frac{\langle \Psi_0 | v_i | \Psi_n \rangle \langle \Psi_n | v_j | \Psi_0 \rangle}{\epsilon_0 - \epsilon_n}$$

energy derivatives and perturbation theory

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$$= \quad 2 \langle \Psi_0 | v_i | \Psi_0'^{j} \rangle$$

energy derivatives and perturbation theory

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$$\begin{aligned} h_{ij} = \left.\frac{\partial^2 E}{\partial \lambda_i \partial \lambda_j}\right|_{\lambda=0} &= 2\sum_n \frac{\langle \Psi_0 | v_i | \Psi_n \rangle \langle \Psi_n | v_j | \Psi_0 \rangle}{\epsilon_0 - \epsilon_n} \\ &= 2\langle \Psi_0 | v_i | \Psi_0'^j \rangle = \int v_i(\mathbf{r})\rho_j'(\mathbf{r})d\mathbf{r} \end{aligned}$$

energy derivatives and perturbation theory

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energy derivatives and perturbation theory

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more about perturbation theory

$$H = H_0 + V'$$

$$\begin{cases} \phi_v^0 \longrightarrow \phi_v^0 + \phi_v' \\ \epsilon_v^0 \longrightarrow \epsilon_v^0 + \epsilon_v' \end{cases}$$

more about perturbation theory

$$H = H_0 + V' \qquad \left\{ \begin{array}{c} \phi_v^0 \longrightarrow \phi_v^0 + \phi_v' \\ \epsilon_v^0 \longrightarrow \epsilon_v^0 + \epsilon_v' \end{array} \right.$$

$$\phi_v' = \sum_{u \neq v} \phi_u^0 \frac{\langle \phi_u^0 | V' | \phi_v^0 \rangle}{\epsilon_v^0 - \epsilon_u^0}$$

more about perturbation theory

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$$(H_0 - \epsilon_v^0)\phi_v' \quad = \quad -\sum_{u \neq v} \phi_u^0 \langle \phi_u^0 | V' | \phi_v^0 \rangle$$

more about perturbation theory

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$$\begin{aligned} (H_0 - \epsilon_v^0)\phi_v' &= -\sum_{u \neq v} \phi_u^0 \langle \phi_u^0 | V' | \phi_v^0 \rangle \\ &= -(1 - P_v) V' | \phi_v^0 \rangle \end{aligned}$$

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more about perturbation theory

$$H = H_0 + V' \qquad \begin{cases} \phi_v^0 \rightarrow \phi_v^0 + \phi_v' \\ \epsilon_v^0 \rightarrow \epsilon_v^0 + \epsilon_v' \end{cases}$$

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$$\boxed{(H_0 - \epsilon_v^0 + \alpha P_v)\bar{\phi}_v' = -P_c V' | \phi_v^0 \rangle}$$

the “2n+1” theorem

$$\Phi = \Phi_0 + \mathcal{O}(\lambda) \Rightarrow E = E_0 + \mathcal{O}(\lambda^2)$$

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$$E = \frac{\langle \Phi_0 + \Phi' | (H_0 + V') | \Phi_0 + \Phi' \rangle}{\langle \Phi_0 + \Phi' | \Phi_0 + \Phi' \rangle} + \mathcal{O}(V'^4)$$

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$$\boxed{E^{(3)} = \langle \Phi' | V' | \Phi' \rangle - \langle \Phi' | \Phi' \rangle \langle \Phi_0 | V' | \Phi_0 \rangle}$$

density-functional perturbation theory

$$V(\mathbf{r}) = V_0(\mathbf{r}) + \sum_i \lambda_i V_i'(\mathbf{r})$$

density-functional perturbation theory

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$$E(\lambda) = \min_n \left(F[n] + \int V_\lambda(\mathbf{r}) n(\mathbf{r}) \right) \quad \int n(\mathbf{r}) d\mathbf{r} = N$$

DFT

density-functional perturbation theory

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$$\frac{\partial E(\lambda)}{\partial \lambda_i} = \int n_\lambda(\mathbf{r}) V_i'(\mathbf{r}) d\mathbf{r}$$ HF

density-functional perturbation theory

$$V(\mathbf{r}) = V_0(\mathbf{r}) + \sum_i \lambda_i V_i'(\mathbf{r})$$

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$$\frac{\partial E(\lambda)}{\partial \lambda_i} = \int n_\lambda(\mathbf{r}) V_i'(\mathbf{r}) d\mathbf{r}$$ HF

$$\boxed{\frac{\partial^2 E(\lambda)}{\partial \lambda_i \partial \lambda_j} = \int \frac{\partial n_\lambda(\mathbf{r})}{\partial \lambda_j} V_i'(\mathbf{r}) d\mathbf{r}}$$ DFPT

dfpt: the equations

DFT

$$V_0(\mathbf{r}) \leftrightarrows n_0(\mathbf{r})$$

dfpt: the equations

DFT

$$V_0(\mathbf{r}) \leftrightarrows n_0(\mathbf{r})$$

$$V_{SCF}(\mathbf{r}) = V_0(\mathbf{r}) + \int \frac{n_0(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu_{xc}(\mathbf{r})$$

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$$\downarrow$$

$$\big(-\Delta + V_{SCF}(\mathbf{r})\big)\phi_v(\mathbf{r}) = \epsilon_v \phi_v(\mathbf{r})$$

dfpt: the equations

DFT

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$$\downarrow$$

$$\boxed{(-\Delta + V_{SCF}(\mathbf{r}))\phi_v(\mathbf{r}) = \epsilon_v \phi_v(\mathbf{r})}$$

$$\downarrow$$

$$n_0(\mathbf{r}) = \sum_{\epsilon_v < E_F} |\phi_v(\mathbf{r})|^2$$

dfpt: the equations

DFT

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$$V_{SCF}(\mathbf{r}) = V_0(\mathbf{r}) + \int \frac{n_0(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu_{xc}(\mathbf{r})$$

$$\boxed{(-\Delta + V_{SCF}(\mathbf{r}))\phi_v(\mathbf{r}) = \epsilon_v \phi_v(\mathbf{r})}$$

$$n_0(\mathbf{r}) = \sum_{\epsilon_v < E_F} |\phi_v(\mathbf{r})|^2$$

DFPT

$$V'(\mathbf{r}) \leftrightarrows n'(\mathbf{r})$$

dfpt: the equations

DFT

DFPT

$$V_0(\mathbf{r}) \leftrightarrows n_0(\mathbf{r})$$

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$$V_{SCF}(\mathbf{r}) = V_0(\mathbf{r}) + \int \frac{n_0(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu_{xc}(\mathbf{r})$$

$$\longrightarrow$$

$$V'_{SCF}(\mathbf{r}) = V'(\mathbf{r}) + \int \frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu'_{xc}(\mathbf{r})$$

$$\downarrow$$

$$\boxed{\left(-\Delta + V_{SCF}(\mathbf{r})\right)\phi_v(\mathbf{r}) = \epsilon_v \phi_v(\mathbf{r})}$$

$$\downarrow$$

$$n_0(\mathbf{r}) = \sum_{\epsilon_v < E_F} |\phi_v(\mathbf{r})|^2$$

dfpt: the equations

DFT

$$V_0(\mathbf{r}) \leftrightarrows n_0(\mathbf{r})$$

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$$\downarrow$$

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DFPT

$$V'(\mathbf{r}) \leftrightarrows n'(\mathbf{r})$$

$$V'_{SCF}(\mathbf{r}) = V'(\mathbf{r}) + \int \frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu'_{xc}(\mathbf{r})$$

$$\downarrow$$

$$\left(-\Delta + V_{SCF}(\mathbf{r}) - \epsilon_v\right)\phi'_v(\mathbf{r}) = -P_c V'_{SCF}\phi_v(\mathbf{r})$$

dfpt: the equations

DFT	DFPT
$V_0(\mathbf{r}) \leftrightarrows n_0(\mathbf{r})$	$V'(\mathbf{r}) \leftrightarrows n'(\mathbf{r})$

$$V_{SCF}(\mathbf{r}) = V_0(\mathbf{r}) + \int \frac{n_0(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu_{xc}(\mathbf{r})$$

$$\big(-\Delta + V_{SCF}(\mathbf{r})\big)\phi_v(\mathbf{r}) = \epsilon_v \phi_v(\mathbf{r})$$

$$n_0(\mathbf{r}) = \sum_{\epsilon_v < E_F} |\phi_v(\mathbf{r})|^2$$

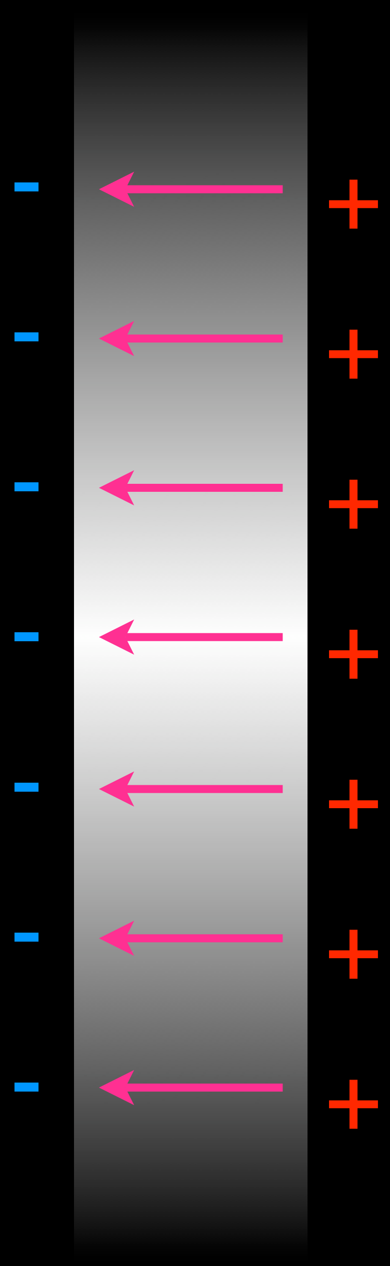
$$V'_{SCF}(\mathbf{r}) = V'(\mathbf{r}) + \int \frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \mu'_{xc}(\mathbf{r})$$

$$\big(-\Delta + V_{SCF}(\mathbf{r}) - \epsilon_v\big)\phi'_v(\mathbf{r}) = -P_c V'_{SCF}\phi_v(\mathbf{r})$$

$$n'(\mathbf{r}) = 2\ \mathrm{Re} \sum_{\epsilon_v < E_F} \phi^*_v(\mathbf{r})\phi'_v(\mathbf{r})$$

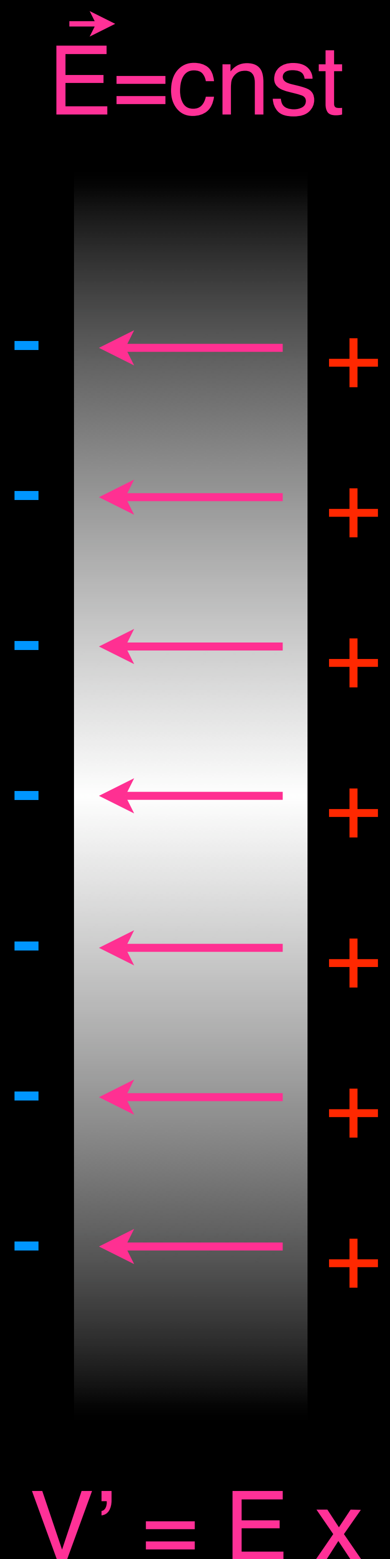
macroscopic electric fields

$\vec{E}$=cnst



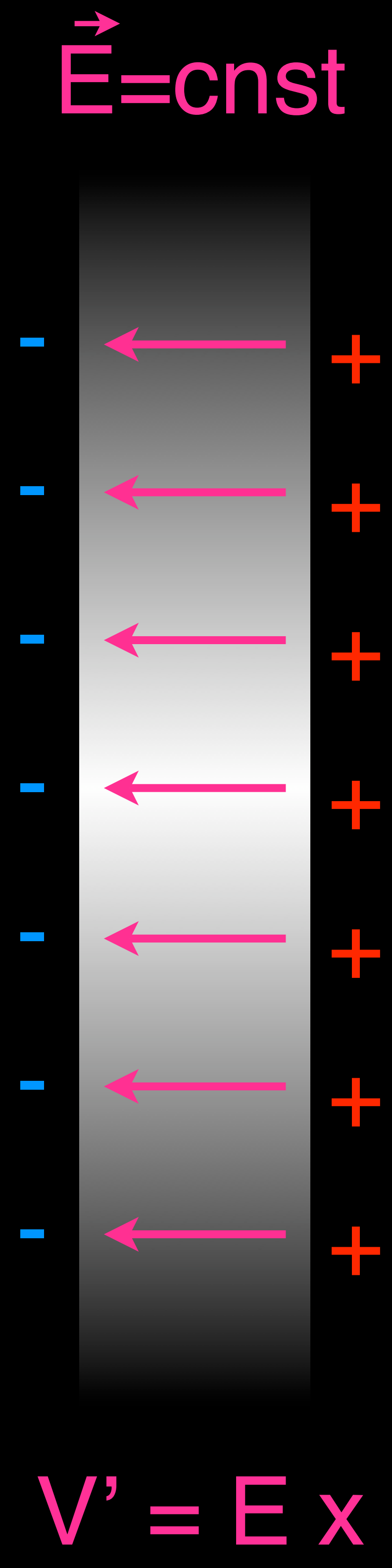
$V' = E\,x$

macroscopic electric fields



$$\phi_v^0(\mathbf{r}) \quad = \quad e^{i\mathbf{k}\cdot\mathbf{r}} u_{v,\mathbf{k}}(\mathbf{r})$$

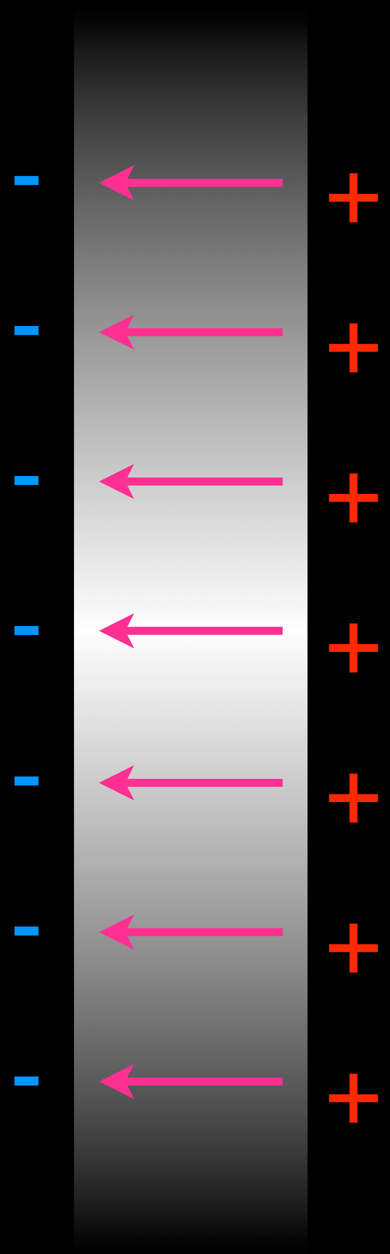
macroscopic electric fields



$$
\begin{aligned}
\phi_v^0(\mathbf{r}) &= \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{v,\mathbf{k}}(\mathbf{r}) \\
V'(\mathbf{r})\phi_v^0(\mathbf{r}) &= ??
\end{aligned}
$$

macroscopic electric fields

$\vec{E}$=cnst

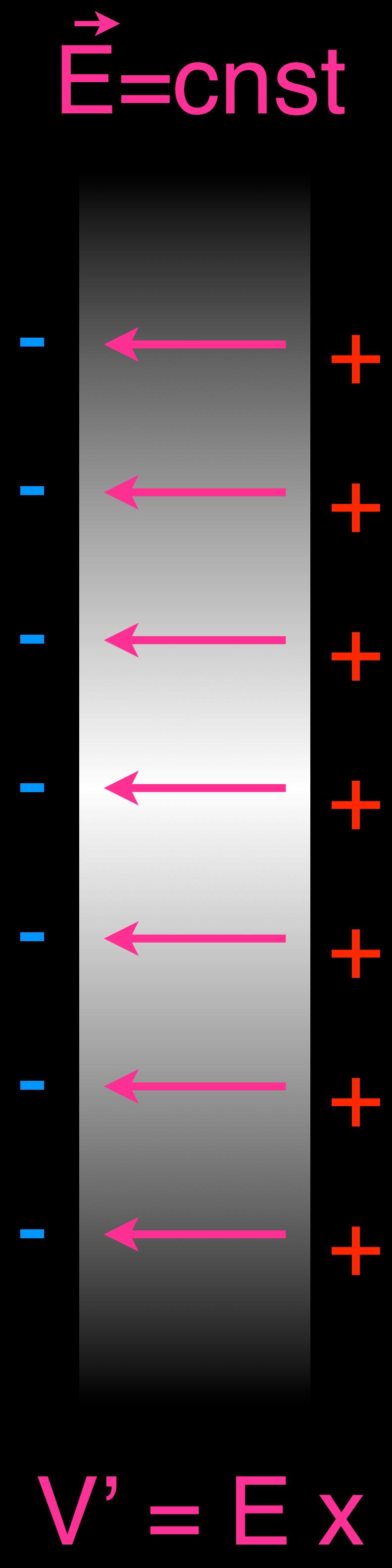


V' = E x

$$\begin{aligned}\phi_v^0(\mathbf{r}) &= \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{v,\mathbf{k}}(\mathbf{r}) \\ V'(\mathbf{r})\phi_v^0(\mathbf{r}) &= ??\end{aligned}$$

$$-P_c V' \phi_v^0 = -E \sum_c \phi_c^0 \langle \phi_c^0 | x | \phi_v^0 \rangle$$

macroscopic electric fields

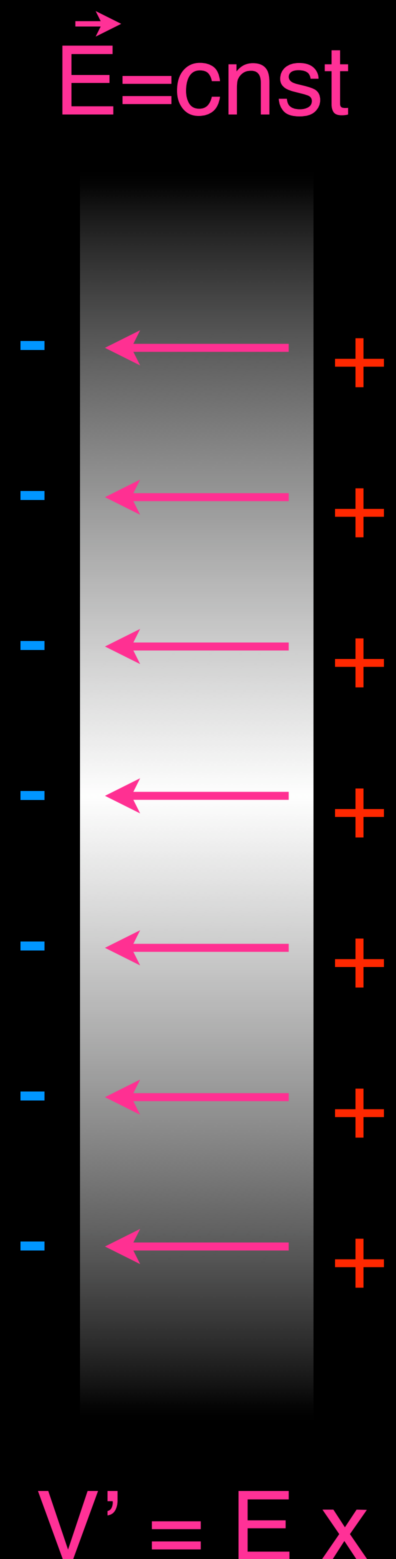


$$
\begin{aligned}
\phi_v^0(\mathbf{r}) &= \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{v,\mathbf{k}}(\mathbf{r}) \\
V'(\mathbf{r})\phi_v^0(\mathbf{r}) &= ??
\end{aligned}
$$

$$
\langle \phi_v^0 | x | \phi_u^0 \rangle = \frac{\langle \phi_v^0 | [H,x] | \phi_u^0 \rangle}{\epsilon_v^0 - \epsilon_u^0} \qquad [H,x] = -\frac{\hbar^2}{m}\frac{\partial}{\partial x} + [H, V_{nl}]
$$

$$
-P_c V' \phi_v^0 = -E \sum_c \phi_c^0 \langle \phi_c^0 | x | \phi_v^0 \rangle
$$

macroscopic electric fields



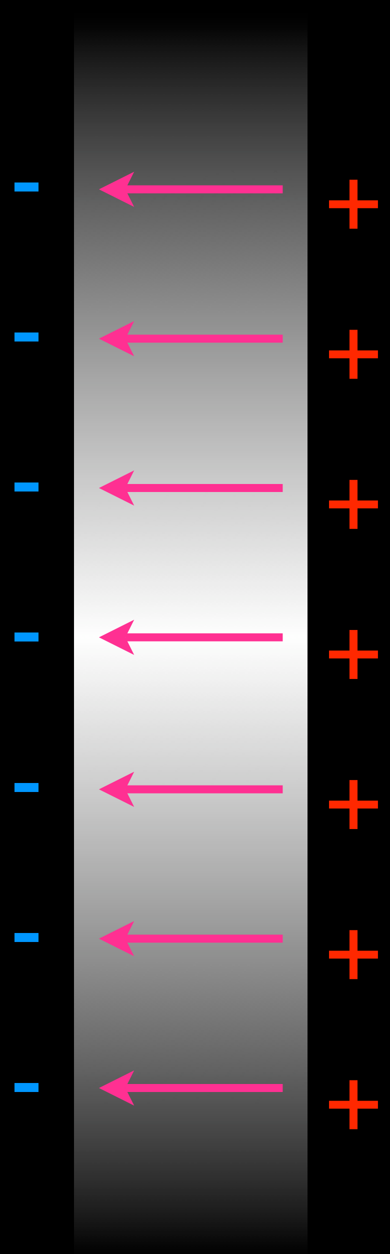
$$\begin{aligned} \phi_v^0(\mathbf{r}) &= \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{v,\mathbf{k}}(\mathbf{r}) \\ V'(\mathbf{r})\phi_v^0(\mathbf{r}) &= ?? \end{aligned}$$

$$\langle\phi_v^0|x|\phi_u^0\rangle = \frac{\langle\phi_v^0|[H,x]|\phi_u^0\rangle}{\epsilon_v^0 - \epsilon_u^0} \qquad [H,x] = -\frac{\hbar^2}{m}\frac{\partial}{\partial x} + [H, V_{nl}]$$

$$\begin{aligned} -P_c V' \phi_v^0 &= -E \sum_c \phi_c^0 \langle\phi_c^0|x|\phi_v^0\rangle \\ &= -E \sum_c \phi_c^0 \frac{\langle\phi_c^0|[H_0,x]|\phi_v^0\rangle}{\epsilon_c^0 - \epsilon_v^0} \equiv \psi_v' \end{aligned}$$

macroscopic electric fields

$\vec{E}$=cnst



V' = E x

$$\begin{aligned}\phi_v^0(\mathbf{r}) &= \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{v,\mathbf{k}}(\mathbf{r}) \\ V'(\mathbf{r})\phi_v^0(\mathbf{r}) &= ??\end{aligned}$$

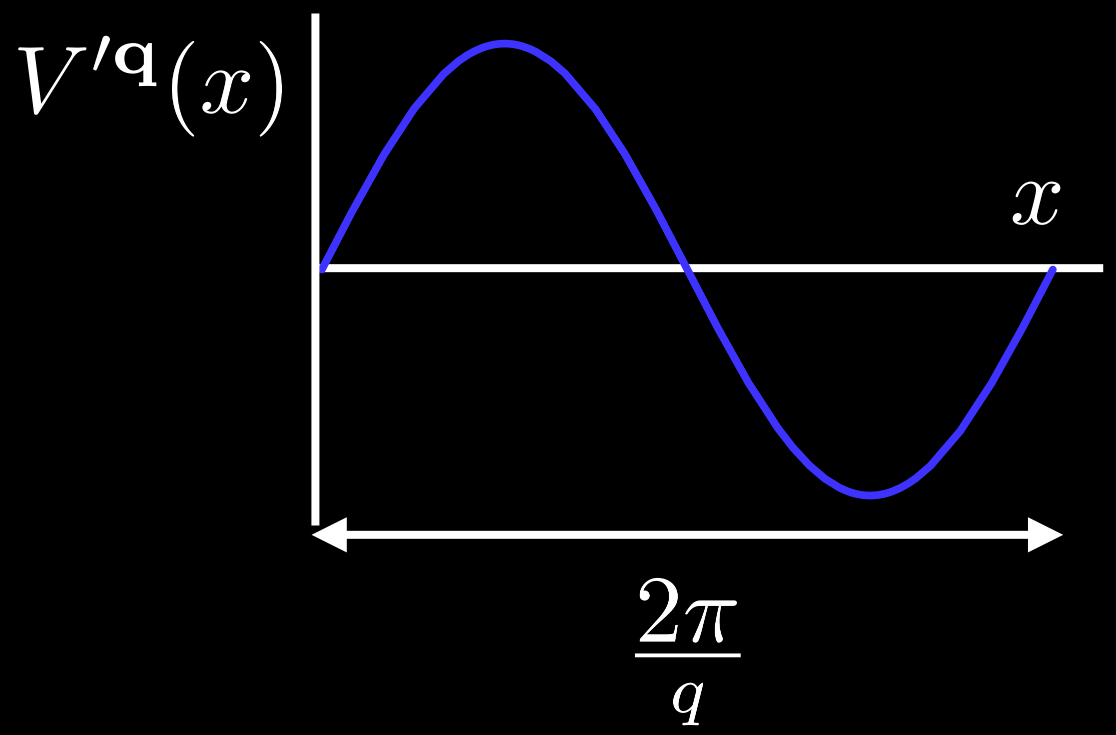
$$\langle\phi_v^0|x|\phi_u^0\rangle = \frac{\langle\phi_v^0|[H,x]|\phi_u^0\rangle}{\epsilon_v^0 - \epsilon_u^0} \qquad [H,x] = -\frac{\hbar^2}{m}\frac{\partial}{\partial x} + [H, V_{nl}]$$

$$\begin{aligned}-P_c V'\phi_v^0 &= -E\sum_c \phi_c^0\langle\phi_c^0|x|\phi_v^0\rangle \\ &= -E\sum_c \phi_c^0 \frac{\langle\phi_c^0|[H_0,x]|\phi_v^0\rangle}{\epsilon_c^0 - \epsilon_v^0} \equiv \psi_v'\end{aligned}$$

$$\boxed{(H_0 - \epsilon_v^0)\psi_v' = -EP_c[H_0, x]\phi_v^0}$$

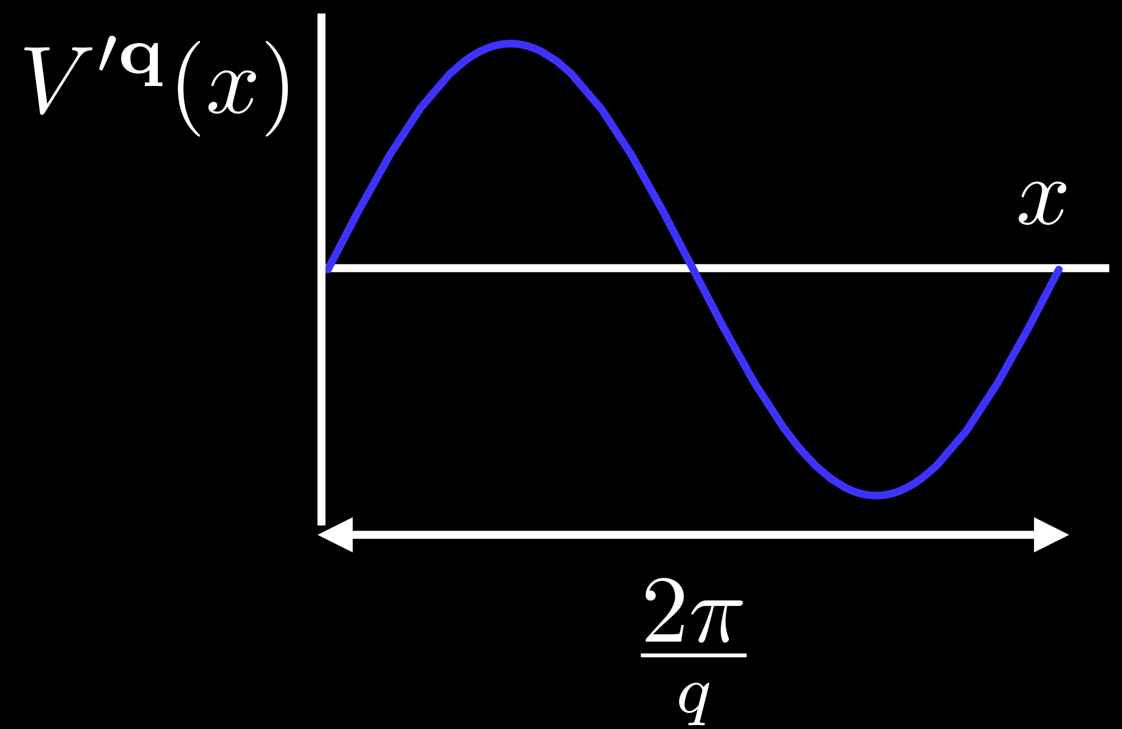
DFPT rhs

monochromatic perturbations



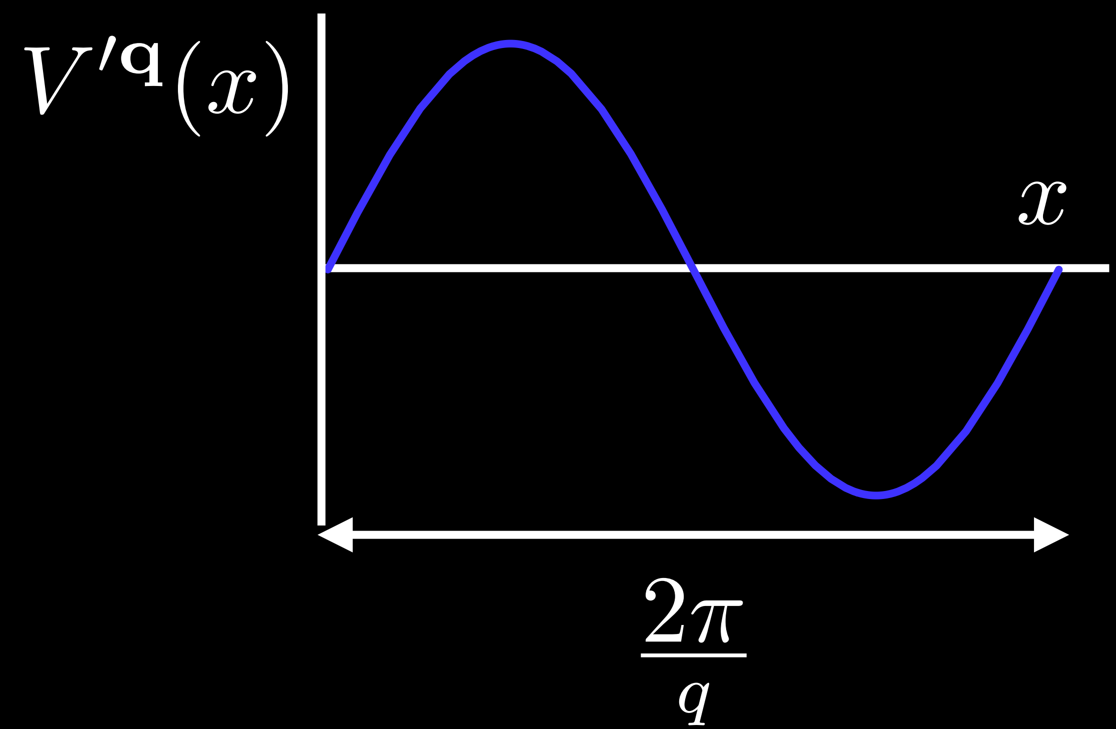
DFPT rhs: $-P_c V'^{\mathbf{q}} \phi_v^{\mathbf{k}}(\mathbf{r})$

monochromatic perturbations



$$\left(H_0 + \alpha P_v^{\mathbf{k}+\mathbf{q}} - \epsilon_v^{\mathbf{k}}\right)\phi_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r}) = -P_c V'^{\mathbf{q}} \phi_v^{\mathbf{k}}(\mathbf{r})$$

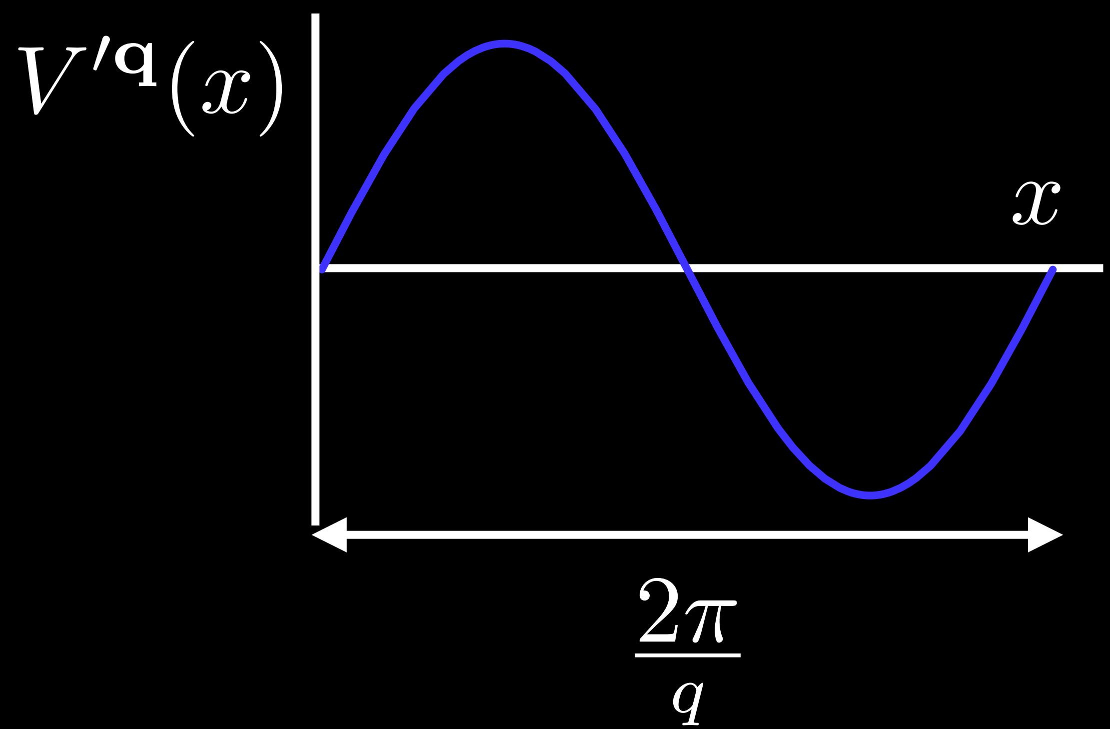
monochromatic perturbations



$$\left(H_0 + \alpha P_v^{\mathbf{k}+\mathbf{q}} - \epsilon_v^{\mathbf{k}}\right)\phi_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r}) = -P_c V'^{\mathbf{q}}\phi_v^{\mathbf{k}}(\mathbf{r})$$

$$n'^{\mathbf{q}}(\mathbf{r}) = \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}} \sum_{v,\mathbf{k}} u_v'^{\mathbf{k}*}(\mathbf{r})\, u_v^{\mathbf{k}+\mathbf{q}}(\mathbf{r})$$

monochromatic perturbations



$$\left(H_0 + \alpha P_v^{\mathbf{k}+\mathbf{q}} - \epsilon_v^{\mathbf{k}}\right)\phi_v'^{\mathbf{k}+\mathbf{q}}(\mathbf{r}) = -P_c V'^{\mathbf{q}}\phi_v^{\mathbf{k}}(\mathbf{r})$$

$$n'^{\mathbf{q}}(\mathbf{r}) = \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}} \sum_{v,\mathbf{k}} u_v'^{\mathbf{k}*}(\mathbf{r}) u_v^{\mathbf{k}+\mathbf{q}}(\mathbf{r})$$

$$V'^{\mathbf{q}}(\mathbf{r}) = V_{ext}'^{\mathbf{q}}(\mathbf{r}) + \int \left(\frac{e^2}{|\mathbf{r}-\mathbf{r}'|} + \kappa_{xc}(\mathbf{r},\mathbf{r}')\right) n'^{\mathbf{q}}(\mathbf{r}')d\mathbf{r}'$$

phonons in polar materials

$$E(\mathbf{u}, \mathsf{E}) = \frac{1}{2} M \omega_0^2 u^2 - \frac{\Omega}{8\pi} \epsilon_\infty \mathsf{E}^2 - e Z^* \mathbf{u} \cdot \mathsf{E}$$

phonons in polar materials

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$$\mathbf{F} \equiv -\frac{\partial E}{\partial \mathbf{u}} = -M\omega_0^2 \mathbf{u} + Z^* \mathsf{E}$$

$$\mathsf{D} \equiv -\frac{4\pi}{\Omega} \frac{\partial E}{\partial \mathsf{E}} = \frac{4\pi}{\Omega} Z^* \mathbf{u} + \epsilon_\infty \mathsf{E}$$

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phonons in polar materials

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phonons in polar materials

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phonons in polar materials

$$E(\mathbf{u}, \mathsf{E}) = \frac{1}{2} M \omega_0^2 u^2 - \frac{\Omega}{8\pi} \epsilon_\infty \mathsf{E}^2 - e Z^* \mathbf{u} \cdot \mathsf{E}$$

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$$\mathbf{F}_T = -M\omega_0^2 \mathbf{u}$$

phonons in polar materials

$$E(\mathbf{u},\mathsf{E}) = \frac{1}{2}M\omega_0^2 u^2 - \frac{\Omega}{8\pi}\epsilon_\infty \mathsf{E}^2 - eZ^*\mathbf{u}\cdot\mathsf{E}$$

$$\mathbf{F} \equiv -\frac{\partial E}{\partial \mathbf{u}} = -M\omega_0^2\mathbf{u} + Z^*\mathsf{E}$$

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$\mathrm{div}\ \mathsf{D} \sim i\mathbf{q}\cdot\mathsf{D} = 0$ $\qquad$ $\mathbf{u}\parallel\mathbf{q} \Rightarrow \mathsf{D} = 0$ $\qquad$ (L)

$$\mathbf{F}_T = -M\omega_0^2\mathbf{u} \qquad \mathbf{F}_L = -M\left(\omega_0^2 + \frac{4\pi Z^*}{M\Omega\epsilon_\infty}\right)\mathbf{u}$$

interatomic force constants

$$\Phi(\mathbf{R}-\mathbf{R}') \quad = \quad -\frac{\partial^2 E}{\partial \mathbf{u}_{\mathbf{R}} \partial \mathbf{u}_{\mathbf{R}'}}$$

interatomic force constants

$$\Phi(\mathbf{R}-\mathbf{R}') = -\frac{\partial^2 E}{\partial \mathbf{u}_{\mathbf{R}} \partial \mathbf{u}_{\mathbf{R}'}}$$

short ranged +
dipole-dipole

interatomic force constants

$$\begin{aligned}\Phi(\mathbf{R}-\mathbf{R}') &= -\frac{\partial^2 E}{\partial \mathbf{u}_{\mathbf{R}} \partial \mathbf{u}_{\mathbf{R}'}} \\ &= \frac{\Omega}{(2\pi)^3} \int \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}')} D(\mathbf{q}) d\mathbf{q}\end{aligned}$$

short ranged + dipole-dipole

interatomic force constants

$$\begin{aligned}\Phi(\mathbf{R}-\mathbf{R}') &= -\frac{\partial^2 E}{\partial \mathbf{u}_{\mathbf{R}} \partial \mathbf{u}_{\mathbf{R}'}} \\ &= \frac{\Omega}{(2\pi)^3} \int \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}')} D(\mathbf{q}) d\mathbf{q}\end{aligned}$$

short ranged + dipole-dipole

- do FFT's
  - \# **q**'s = # **R**'s
  - remove singularities in D(q)

interatomic force constants

$$\Phi(\mathbf{R}-\mathbf{R}') = -\frac{\partial^2 E}{\partial \mathbf{u}_{\mathbf{R}} \partial \mathbf{u}_{\mathbf{R}'}}$$

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short ranged +
dipole-dipole

- do FFT's
    - # **q**'s = # **R**'s
    - remove singularities in D(q)
- store information

interatomic force constants

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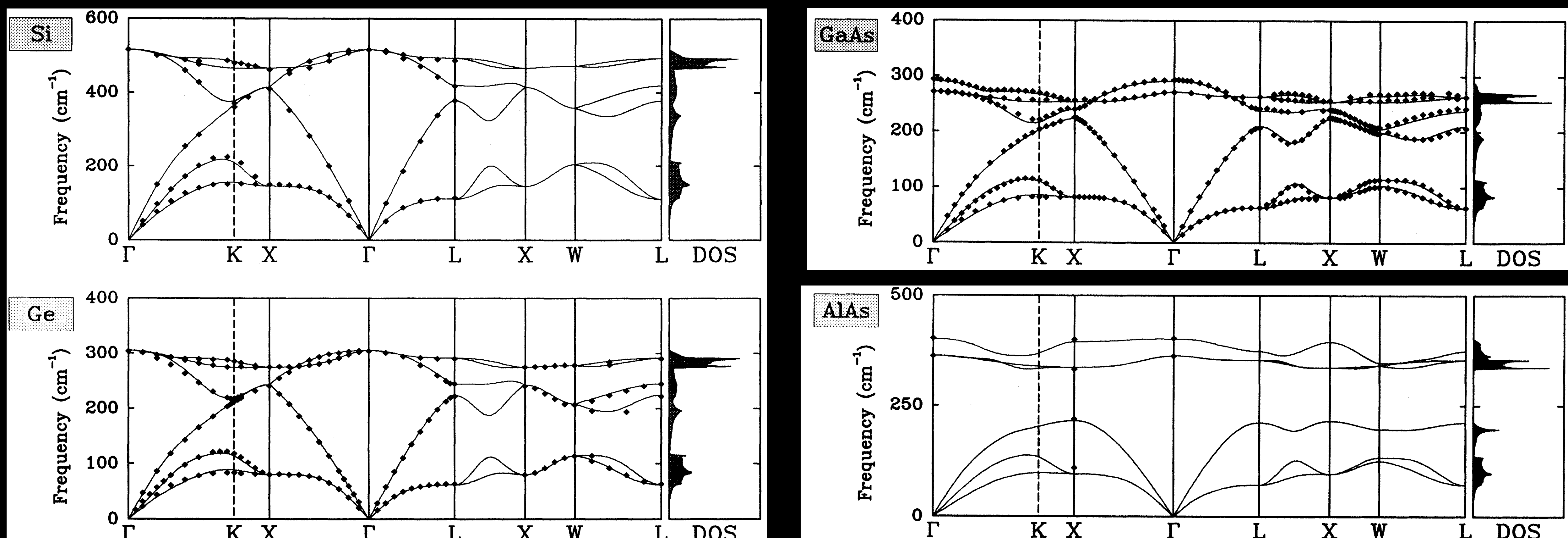
short ranged +
dipole-dipole

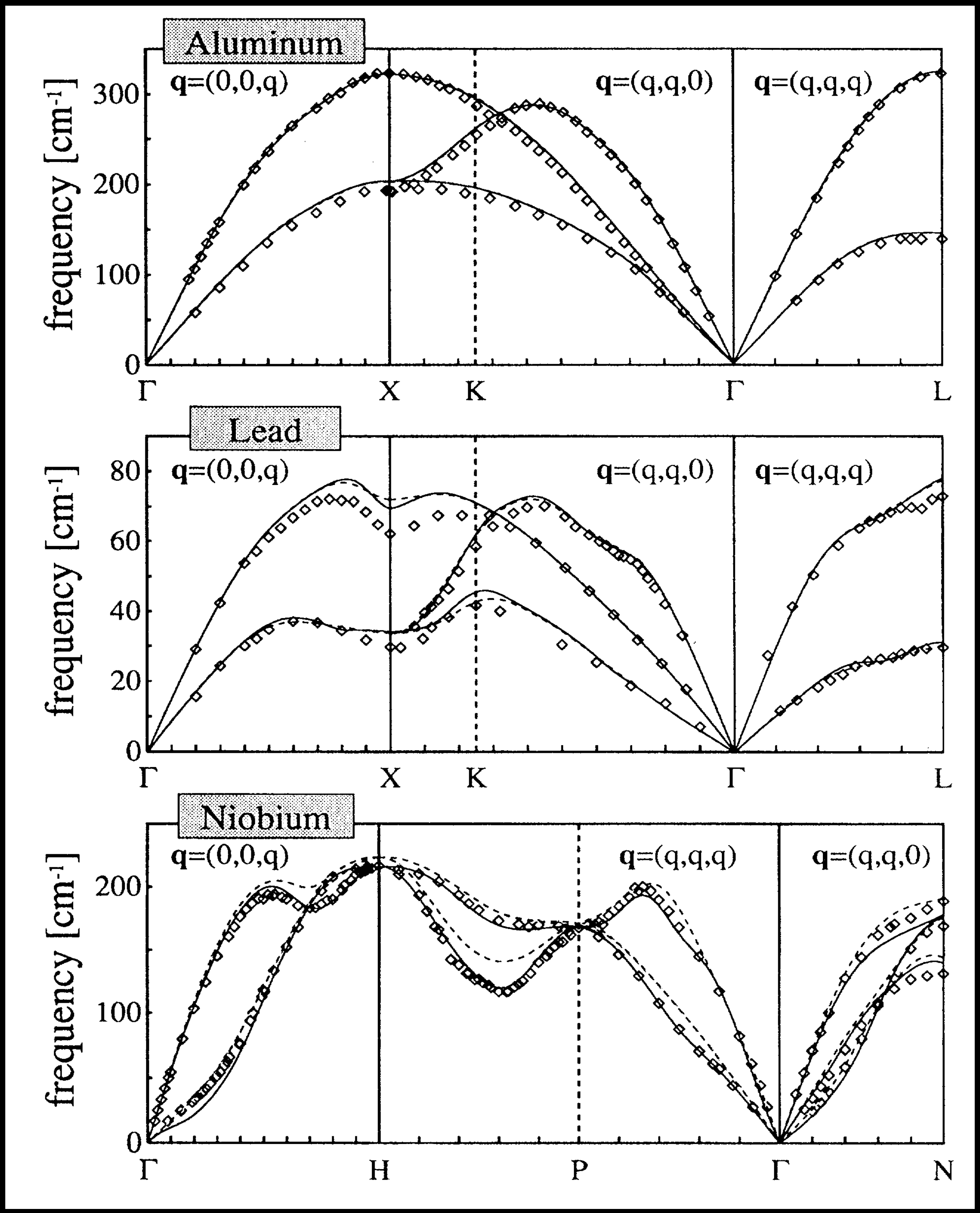
- do FFT's
  - # **q**'s = # **R**'s
  - remove singularities in D(q)
- store information
- interpolate phonon bands

phonons from DFPT



P. Giannozzi, S. de Gironcoli, P. Pavone, and S. Baroni, Phys. Rev. B **43**, 7231 (1991)

phonons from DFPT



S. de Gironcoli, Phys. Rev. B **51**, 6773 (1995)

applications done so far

- Dielectric properties
- Piezoelectric properties
- Elastic properties
- Phonon in crystals and alloys
- Phonon at surfaces, interfaces, super-lattices, and nano-structures
- Raman and infrared activities
- Anharmonic couplings and vibrational line widths
- Mode softening and structural transitions
- Electron-phonon interaction and superconductivity
- Thermal expansion
- Isotopic effects on structural and dynamical properties
- Thermo-elasticity and other thermal properties of minerals
- …

S. Baroni, A. Dal Corso, S. de Gironcoli, and P. Giannozzi, Phonons and related crystal properties from density-functional perturbation theory, Rev. Mod. Phys. **73**, 515 (2001)

these slides at
http://stefano.baroni.me/presentations