Anyagtudomány
Röntgendiffrakció I

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Maxwell egyenletek

$$div\underline{D} = \rho \qquad \underline{D} = \epsilon_0 \underline{E} + \underline{P}$$

$$\rho = 0 \qquad div\underline{E} = \frac{\rho_0}{\epsilon_0} = -\frac{1}{\epsilon_0} div\underline{P}$$

$$div\underline{B} = 0;$$

$$rot\underline{E} = -\underline{\dot{B}}$$

$$rot\underline{H} = \underline{j} + \underline{\dot{D}} \qquad \underline{H} = \frac{\underline{B}}{\mu_0} - \underline{M}$$

$$\underline{j} = 0 \qquad rot\underline{B} - \epsilon_0\mu_0\underline{\dot{E}} = \mu_0\left(rot\underline{M} + \underline{\dot{P}}\right) = \mu_0\underline{j}_0$$

Potenciálok

Bevezetve

$$\underline{B} = rot\underline{A} \qquad \underline{E} = -grad\phi - \dot{\underline{A}}$$

Lorentz mérték

$$div\underline{A} + \epsilon_0\mu_0\dot{\phi} = 0$$

$$\triangle\underline{A} - \epsilon_0\mu_0\ddot{\underline{A}} = -\mu_0\underline{j}_0 = -\mu_0\left(rot\underline{M} + \dot{\underline{P}}\right)$$

$$\triangle\phi - \epsilon_0\mu_0\ddot{\phi} = -\frac{\rho_0}{\epsilon_0} = \frac{1}{\epsilon_0}div\underline{P}$$

Hertz vektorok

$$\underline{A} = \mu_0(\dot{\underline{\Pi}}_e + rot\underline{\Pi}_m)$$

$$\phi = -\frac{1}{\epsilon_0}div\underline{\Pi}_e$$

Feltesszük $\underline{M} = 0 \longrightarrow \underline{\Pi}_m = 0$

Hertz vektor

$$\triangle \underline{\Pi}_e - \frac{1}{c^2}\ddot{\underline{\Pi}}_e = -\underline{P}(\underline{E})$$

$$\underline{E} = \frac{1}{\epsilon_0} grad\ div \underline{\Pi}_e - \mu_0 \ddot{\underline{\Pi}}_e$$

Az elektron mozgásegyenlete

$$m\ddot{\underline{r}} = -\omega_0^2 m\underline{r} - \lambda\dot{\underline{r}} - e\underline{E}_0 e^{i\omega t}$$

$$\underline{r} = \frac{-e\underline{E}_0}{m(\omega_0^2 - \omega^2) + i\lambda\omega} e^{i\omega t}$$

$$\underline{p} = -e\underline{r} = \frac{e^2\underline{E}_0}{m(\omega_0^2 - \omega^2) + i\lambda\omega} e^{i\omega t}$$

$$\underline{P}dV == \frac{\rho(\underline{r})e^2}{m(\omega_0^2 - \omega^2) + i\lambda\omega}\underline{E}dV$$

$$\chi = \frac{\rho(\underline{r})}{\epsilon_0}\frac{e^2}{m(\omega_0^2 - \omega^2) + i\lambda\omega}$$

röntgenre $\omega_0 << \omega$, λ kicsi

Szórása egyenlete

$$\chi = \frac{\rho(\underline{r})}{\epsilon_0}\frac{e^2}{m\omega^2} = \rho(\underline{r})\frac{e^2}{4\pi^2 c^2 \epsilon_0}\lambda_e^2$$

A Szórás egyenlete

$$\triangle \underline{\Pi}_e - \frac{1}{c^2}\ddot{\underline{\Pi}}_e = -\beta\rho(\underline{r})\left[\frac{1}{\epsilon_0} grad\ div \underline{\Pi}_e - \mu_0 \ddot{\underline{\Pi}}_e\right]$$

Periodikus megoldás $\underline{\Pi}(t) = \underline{\Pi}_\alpha e^{i\omega t}$

$$\triangle \underline{\Pi}_e + k^2 \underline{\Pi}_e = -\beta\rho(\underline{r})\left[\frac{1}{\epsilon_0} grad\ div \underline{\Pi}_e + \mu_0 \omega^2 \underline{\Pi}_e\right]$$

Perturbáció számítás ρ szerinti sor

$$\underline{\Pi}_e = \underline{\Pi}_0 + \underline{\Pi}_1 + \ldots$$

$$\triangle \underline{\Pi}_0 + k^2 \underline{\Pi}_0 = 0 \ \longrightarrow\ \underline{\Pi}_0 = \underline{A}_0 e^{i\underline{kr}}$$

$$\triangle \underline{\mathit{\Pi}}_1 + k^2 \underline{\mathit{\Pi}}_1 = -\beta\rho(\underline{r}) \left[\frac{1}{\epsilon_0} grad\ div \underline{\mathit{\Pi}}_0 + \mu_0 \omega^2 \underline{\mathit{\Pi}}_0 \right]$$

Inhomogén Helmholtz egyenlet

$$\triangle \underline{\mathit{\Pi}}_1 + k^2 \underline{\mathit{\Pi}}_1 = -\rho(\underline{r}) \underline{Z}(\underline{k}) e^{i\underline{k}\underline{r}}$$

Green függvény

$$\triangle G + k^2 G = \delta(\underline{r})$$

$$\frac{1}{r} \frac{\partial^2}{\partial r^2} (rG) + k^2 G = \delta(\underline{r})$$

Gömbhullám

$$G = \frac{e^{i|\underline{k}||\underline{r}|}}{4\pi r}$$

Kinematikus szórása

$$\triangle\psi + k^2\psi = -\rho(\underline{r})\psi_0(\underline{k})e^{i\underline{k}\underline{r}}$$

Megoldás (Huygens-Fresnel-elv)

$$\psi(\underline{r}) = -\int \rho(\underline{r}')e^{i\underline{k}\underline{r}'}\psi_0 \frac{e^{i|\underline{k}||\underline{r}-\underline{r}'|}}{4\pi|\underline{r}-\underline{r}'|}dV'$$

ha (Fraunhoffer elrendezés)

$$r >> r' \quad |\underline{r}-\underline{r}'| \approx |\underline{r}| - \frac{\underline{r}}{|\underline{r}|}\underline{r}' = |\underline{r}| - \underline{n}\underline{r}'$$

ekkor bevezetve $\underline{k}_o = \underline{n}|\underline{k}_i|$

$$\psi(\underline{r}) = -\int \rho(\underline{r}')e^{i(\underline{k}_i-\underline{k}_o)\underline{r}'}dV'\psi_0\frac{e^{i|\underline{k}||\underline{r}|}}{4\pi r}$$

Szórási amplitúdó ($\underline{\kappa} = \underline{k}_i - \underline{k}_o$)

$$A(\underline{\kappa}) = -\int \rho(\underline{r})e^{i\underline{\kappa}\underline{r}}dV$$

Szórt intenzitás

Poynting vektor

$$\underline{S} = \underline{E} \times \underline{H}$$

elektromágneses hullámba $|\underline{H}| \propto |\underline{E}|$

$$I = |\underline{S}| \propto |\underline{E}|^2 \propto A(\underline{\kappa})A^*(\underline{\kappa})$$

$$I(\underline{\kappa}) \propto |A(\underline{\kappa})|^2$$