① Fri. 9/20/02

<u>Summary</u>.

$$\nabla\cdot\vec{e} = \frac{1}{\varepsilon_0}\eta \qquad \vec{E} = \langle\vec{e}\rangle \qquad \nabla\cdot\vec{E} = \frac{1}{\varepsilon_0}\langle\eta\rangle$$

$$\nabla\times\vec{e} + \frac{\partial\vec{b}}{\partial t} = 0 \qquad \vec{B} = \langle\vec{b}\rangle \qquad \nabla\times\vec{E} + \frac{\partial\vec{B}}{\partial t} = 0$$

$$\nabla\cdot\vec{b} = 0 \qquad \nabla\cdot\vec{B} = 0$$

$$\nabla\times\vec{b} - \varepsilon_0\mu_0\frac{\partial\vec{e}}{\partial t} = \mu_0\vec{j} \qquad \nabla\times\vec{B} - \varepsilon_0\mu_0\frac{\partial\vec{E}}{\partial t} = \langle\vec{j}\rangle.$$

$$\langle F(\vec{x})\rangle = \int d^3\vec{x}'\; F(\vec{x}-\vec{x}')\; f(\vec{x}')$$

$f(\vec{x}) = f(-\vec{x}) =$ window fn. scale $= L =$ mesoscopic.

So, $\langle\ \rangle$ commutes with ∇, $\frac{\partial}{\partial t}$.

Now define
$$\vec{E} = \langle\vec{e}\rangle$$
$$\vec{B} = \langle\vec{b}\rangle.$$

immediately obtain,
$$\nabla\cdot\vec{E} = \frac{1}{\varepsilon_0}\langle\eta\rangle$$
$$\nabla\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$
$$\nabla\cdot\vec{B} = 0$$
$$\nabla\times\vec{B} = \mu_0\langle\vec{j}\rangle + \varepsilon_0\mu_0\frac{\partial\vec{E}}{\partial t}.$$

So we need to work out $\langle\eta\rangle$ and $\langle\vec{j}\rangle$. Do $\langle\eta\rangle$ first.

Adopt microscopic model. charges = free + bound ~~(don't call them Bound). 2 (get)~~.

Free = conduction electrons + any other external charges.
Bound ~~[illegible]~~. = charges bound to molecules.

Write $\eta = \eta_f + \eta_b$

$$\eta_f(\vec{x}) = \sum_j q_{fj}\,\delta(\vec{x}-\vec{x}_{fj})$$

q_{fj} = j-th free chg.
$\vec{x}_{fj}$ = loc'n of j-th free chg.

$$\langle\eta_f\rangle = \sum_j q_{fj}\int d^3x'\ \delta(\vec{x}-\vec{x}'-\vec{x}_{fj})\,f(\vec{x}')$$
$$= \sum_j q_{fj}\,f(\vec{x}-\vec{x}_{fj})$$

Rule: To avg, replace δ by f.

$$\equiv \rho_f.$$

~~η_b~~

$$\eta_b = \sum_n \eta_{bn}$$

$$\eta_{bn}(\vec{x}) = \sum_j q_{nj}\, \delta(\vec{x} - \vec{x}_n - \vec{x}_{nj})$$

n = label / index of molecules

$\vec{x}_n$ = COM of n-th molecule

$\vec{x}_{nj}$ = posn of j-th chg in molecule n rel. to $\vec{x}_n$

q_{nj} = chg of j-th particle in molecule.

$$\langle \eta_b(\vec{x}) \rangle = \sum_n \langle \eta_{bn}(\vec{x}) \rangle$$

$$= \sum_n \sum_j q_{nj}\, f(\vec{x} - \vec{x}_n - \vec{x}_{nj}).$$

Now, $|\vec{x}_{nj}| \ll L$ ratio maybe $\frac{1}{100}$. So expand f:

$$\langle \eta_b(\vec{x}) \rangle = \sum_n \sum_j q_{nj} \Big[f(\vec{x} - \vec{x}_n) - \vec{x}_{nj} \cdot \nabla f(\vec{x} - \vec{x}_n) + \tfrac{1}{2} \underbrace{\vec{x}_{nj}\, \vec{x}_{nj} : \nabla\nabla f}_{x^\alpha_{nj}\, x^\beta_{nj}\, \frac{\partial^2 f}{\partial x_\alpha \partial x_\beta}} + \dots \Big]$$

In 1st term, let $q_n = \sum_j q_{jn}$ = chg. on n-th molecule.

2nd term, $\vec{p}_n = \sum_j q_{jn}\, \vec{x}_{jn}$ = dipole mom. of n-th molec.

3rd term, $t_n^{\alpha\beta} = \sum_j q_{jn}\, x^\alpha_{jn}\, x^\beta_{jn}$ = a tensor, 2nd moment, related to quad. mom. (but not traceless).

$\alpha, \beta = 1, 2, 3$

$$\text{1st term} = \sum_n q_n\, f(\vec{x} - \vec{x}_n) = \Big\langle \sum_n q_n\, \delta(\vec{x} - \vec{x}_n) \Big\rangle \equiv \rho_m$$

= molecular chg. density.

$$\text{2nd term} = -\sum_n \sum_j q_{nj}\, \vec{x}_{nj} \cdot \nabla f(\vec{x}-\vec{x}_n)$$

$$= -\sum_n \vec{p}_n \cdot \nabla f(\vec{x}-\vec{x}_n) = -\nabla\cdot\vec{P}$$

$$\text{where} \quad \vec{P} = \sum_n \vec{p}_n\, f(\vec{x}-\vec{x}_n) = \left\langle \sum_n \vec{p}_n\, \delta(\vec{x}-\vec{x}_n) \right\rangle$$

(defn of macroscopic polarization).

$$\text{3rd term} = \frac{1}{2} \sum_n t_n^{\alpha\beta} \frac{\partial^2 f}{\partial x_\alpha \partial x_\beta}(\vec{x}-\vec{x}_n) = \frac{1}{2} \frac{\partial^2}{\partial x_\alpha \partial x_\beta} T_{\alpha\beta},$$

$$\text{where} \quad T_{\alpha\beta} = \sum_n t_n^{\alpha\beta}\, f(\vec{x}-\vec{x}_n) = \left\langle \sum_n t_n^{\alpha\beta}\, \delta(\vec{x}-\vec{x}_n) \right\rangle$$

altogether,

$$\nabla\cdot\vec{E} = \frac{1}{\varepsilon_0}\langle\eta\rangle = \frac{1}{\varepsilon_0}\left(\langle\eta_f\rangle + \langle\eta_b\rangle\right)$$

$\frac{1}{2}\nabla\cdot\vec{R}$

$$= \frac{1}{\varepsilon_0}\left[\rho_f + \rho_m - \nabla\cdot\vec{P} + \underbrace{\frac{1}{2} T_{\alpha\beta,\alpha\beta}}_{} + \cdots \right]$$

small correction,
order $\left(\frac{r_{atom}}{L}\right)$ compared to $\nabla\cdot\vec{P}$.

keep it anyway, need it for analysis of $\vec{J}$.

$$\text{Anyway define} \quad R_\alpha = \frac{\partial T_{\alpha\beta}}{\partial x_\beta},$$

$$\text{define} \quad \vec{D} = \cancel{\varepsilon_0 \vec{E}}\ \varepsilon_0\vec{E} + \vec{P} + \frac{1}{2}\vec{R} + \cdots$$

$$\text{and you get} \quad \boxed{\nabla\cdot\vec{D} = \rho_f + \rho_m}$$

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Similarly, when we compute $\langle \vec{j} \rangle$ we get...

$$\boxed{\nabla \times \vec{H} = \vec{J}_f + \vec{J}_m + \frac{\partial \vec{D}}{\partial t},}$$

where:

$$\vec{J}_f(\vec{x}) = \sum_j q_{fj}\, \vec{v}_{fj}\, f(\vec{x} - \vec{x}_{fj}) = \left\langle \sum_j q_{fj}\, \vec{v}_{fj}\, \delta(\vec{x} - \vec{x}_{fj}) \right\rangle$$

$= $ free current. , $\vec{v}_{f_j} = \dot{\vec{x}}_{fj}$

$$\vec{J}_m(\vec{x}) = \sum_n q_n \vec{v}_n f(\vec{x} - \vec{x}_n) = \left\langle \sum_n q_n \vec{v}_n\, \delta(\vec{x} - \vec{x}_n) \right\rangle$$

$=$ molecular current, $\vec{v}_n = \dot{\vec{x}}_n$

$=$ current due to motion of COM's of molecules.

$$\vec{H} = \frac{\vec{B}}{\mu_0} - \vec{M} - \underbrace{\sum_n (\vec{p}_n \times \vec{v}_n)\, f(\vec{x} - \vec{x}_n)}_{\Big\downarrow \; \left\langle \sum_n (\vec{p}_n \times \vec{v}_n)\, \delta(\vec{x} - \vec{x}_n) \right\rangle} \leftarrow \text{extra contribution to magnetization.}$$

$$\vec{M}(\vec{x}) = \sum_n \vec{m}_n f(\vec{x} - \vec{x}_n) = \left\langle \sum_n \vec{m}_n\, \delta(\vec{x} - \vec{x}_n) \right\rangle$$

$$\text{where } \vec{m}_n = \frac{1}{2} \sum_j q_{nj} (\vec{x}_{nj} \times \vec{v}_{nj})$$

Comments:

① In dielectric, ρ_m, $\vec{J}_m = 0$ because $q_n = 0$ (molecules neutral), but here we allow for charge, current of ions.

② Extra contribution to magnetization usu. small, unless matter is in bulk motion.