Currents, Conductivity, and sum rule

$$H = -\sum_{\substack{jk,\\ s}} t_{jk} \hat{c}^{+}_{js} \hat{c}_{ks} + U \sum_{\ell} \hat{n}_{\ell\downarrow} \hat{n}_{\ell\uparrow}$$

HM, allowing for long-distance hopping

Next, write down the centre-of-mass position,

$$\hat{X}_{cm} = \frac{1}{N} \sum_{\ell s} x_{\ell} \hat{n}_{\ell s}$$ where $x = \ell a_L$ in 1D

(drop spin indices for simplicity)

we define the total current $\hat{J}_x = N \frac{d}{dt} \hat{X}_{cm}$

$$\hat{J} = \frac{iN}{\hbar} [\hat{H}, \hat{X}_{cm}]$$

$$= \frac{iN}{\hbar} [\hat{H}_0, \hat{X}_{cm}]$$ because $[X_{cm}, \hat{H}_U] = 0$

(and also X_{cm}, V_{trap} commute...)

$$= -\frac{iN}{\hbar} \sum_{\langle jk \rangle} \sum_{\ell} [t_{jk} \hat{c}^{+}_{j} \hat{c}_{k}, x_{\ell} \hat{c}^{+}_{\ell} \hat{c}_{\ell}]$$

One can show that $[\hat{c}^{+}_{a} \hat{c}_{b}, \hat{n}_{d}] = (\delta_{bd} - \delta_{ad}) \hat{c}^{+}_{a} \hat{c}_{b}$,

$[n_a, \hat{c}^{+}_{c} \hat{c}_{d}] = (\delta_{ac} - \delta_{ad}) \hat{c}^{+}_{c} \hat{c}_{d}$

so ...

$$= -\frac{i}{\hbar} \sum_{\substack{jk\\ s}} t_{jk} (x_k - x_j) \hat{c}^{+}_{j,s} \hat{c}_{k,s}$$

Applied to TB HM, only $t_{jk} = t\, \delta_{j,k\pm 1}$, so

$$\hat{J} = -\frac{i t a_L}{\hbar} \sum_{\ell, s} (\hat{c}^{+}_{\ell} \hat{c}_{\ell+1} - \hat{c}^{+}_{\ell+1} \hat{c}_{\ell})$$

Current is almost like the tunnelling $\hat{H}_0$ itself, but with an extra i, so that we could write

$$\hat{J} = \frac{t q_L}{\hbar} \sum_{\ell} i \hat{c}_{\ell}^{+} \hat{c}_{\ell+1} + h.c.$$

The local current, $j_{\ell\uparrow} = -it \, c_{\ell\uparrow}^{+} c_{\ell+1,\uparrow} + h.c.$

satisfies the continuity equation

$$\dot{n}_{m\uparrow} + j_{m\uparrow} - j_{m-1,\uparrow} = 0$$

where $\dot{n}_{m\uparrow} = i/\hbar [H, n_{m\uparrow}]$, by following the same steps as above, but locally.

One defines the conductivity as the ratio

$$\sigma(\omega) = \frac{J(\omega)}{F(\omega)}$$

J: particles · m/s
F: J/m

and more generally, one can have an off-diagonal push & response, e.g.

$$\sigma_{\alpha\beta}(\omega) = \frac{J_\alpha(\omega)}{F_\beta(\omega)}$$

The current in a cold atom experiment can be determined by watching the cm dynamics,

eg some $R_{cm} = A \cos(\omega t - \phi)$

response amplitude & phase

drive frequency

since $J = N \frac{dR_{cm}}{dt}$, $J = -A\omega \sin(\omega t - \phi)$

$$= 2\,\mathrm{Re}\Big\{\underbrace{\frac{iA\omega}{2} e^{-i\omega t} e^{i\phi}}\Big\}$$

$$J_\alpha(\omega) = \frac{iA_\alpha\omega}{2} e^{i\phi_\alpha}$$

with $\begin{cases} F = F_{0\beta}\cos\omega t \\ \;\; = 2\,\mathrm{Re}\left\{\frac{F_{0\beta}}{2} e^{-i\omega t}\right\} \end{cases}$

Then $\sigma = \frac{J_\alpha(\omega)}{F_\beta(\omega)} = \frac{iA_\alpha\omega\, e^{i\phi_\alpha}}{F_\beta}$

For observed response of cm dynamics,

$$\langle R_\alpha(t)\rangle = \sigma_{\alpha\beta}\frac{iF_{0\beta}}{2\omega N} e^{-i\omega t} + c.c.$$

$$J_\alpha(t) = \sigma_{\alpha\beta}\frac{F_{0\beta}}{2} e^{-i\omega t} + c.c.$$

Now, how does such a current get created, with an external force? Apply a perturbative force F, and ask for what happens to a

pt: $\hat{H} = \hat{H}_0 + \hat{H}_1(t)$

$$|\psi(t)\rangle = \sum \gamma_n \underbrace{e^{-iE_nt/\hbar}}_{\text{or } e^{-i\omega_n t}} |n\rangle \quad , \quad \hat{H}_0|n\rangle = E_n|n\rangle$$

$$i\hbar \frac{d}{dt}\gamma_n = \sum_{n'} \langle n|\hat{H}_1(t)|n'\rangle \, e^{i(E_n - E_{n'})t/\hbar}\gamma_{n'}$$

$$= \langle n|\hat{H}_1(t)|0\rangle \, e^{i\omega_{n0}t} \quad \text{if } \gamma_0 = 1, \; \& \; \omega_{n0} \equiv \frac{E_n - E_0}{\hbar}$$

Now choose an $\hat{H}_1(t) = -F \underbrace{\cos(\omega t)\, e^{\varepsilon t}}_{\frac{1}{2}\left(e^{-i\omega t + \varepsilon t} + e^{+i\omega t + \varepsilon t}\right)} \underbrace{\sum_{\ell, s} x_\ell \hat{n}_{\ell, s}}_{N \hat{X}_{cm}}$

So $i\hbar \frac{d}{dt}\gamma_n = \langle \hat{X}_{cm} \rangle_{n0} \frac{-FN}{2} \left(e^{i(\omega + \omega_{n0} - i\varepsilon)t} + e^{i(-\omega + \omega_{n0} - i\varepsilon)t} \right)$

integrate from $-\infty \to$ some time t,

$$\gamma_n(t) = \frac{-FN}{2i\hbar} \langle \hat{X}_{cm} \rangle_{n0} \int_{-\infty}^{t} dt' \left[e^{i(\omega_{n0} + \omega - i\varepsilon)t} + e^{i(\omega_{n0} - \omega - i\varepsilon)t} \right]$$

$$= \frac{FN}{2\hbar} e^{i\omega_{n0}t} \langle \hat{X}_{cm} \rangle_{n0} \left(\frac{e^{i\omega t}}{\omega + \omega_{n0} - i0^+} + \frac{e^{-i\omega t}}{-\omega + \omega_{n0} - i0^+} \right)$$

The response in position, R_α, is to first-order

$$\langle R_\alpha \rangle = \langle \psi | \hat{R}_\alpha | \psi \rangle$$
$$= \left(\langle \psi_0 | + \sum_n \gamma_n^* \langle n | e^{i\omega_n t} \right) \hat{R}_\alpha \left(|\psi_0\rangle + \sum_n \gamma_n e^{-i\omega_n t} |n\rangle \right)$$

so, keeping terms only 1^{st} order in F, the displacement is

$$\langle R_\alpha \rangle - \langle R_\alpha \rangle_0 \approx \sum_n \langle 0 | \hat{R}_\alpha | n \rangle \gamma_n e^{-i\omega_{n0} t} + \langle n | \hat{R}_\alpha | 0 \rangle \gamma_0^* e^{i\omega_n t}$$

putting in our results for $\gamma_n(t)$, from TDPT,

$$\Delta \langle R_\alpha \rangle = \frac{F_\beta N}{2\hbar} e^{i\omega t} \sum_n \frac{\langle \hat{R}_\alpha \rangle_{0n} \langle \hat{R}_\beta \rangle_{n0}}{\omega + \omega_{n0} - i0^+} + \frac{\langle R_\alpha \rangle_{n0} \langle R_\beta \rangle_{0n}}{-\omega + \omega_{n0} + i0^+} + c.c.$$

for current, one takes the time derivative of the position. $J_\alpha = \frac{d}{dt} \langle R_\alpha \rangle$,

$$J_\alpha(t) = \frac{i\omega F_\beta N}{2\hbar} e^{i\omega t} \sum_n \cdots\cdots \quad + c.c.$$

comparing this to $J_\alpha(t) = \sigma_{\alpha\beta} \frac{F_\beta}{2} e^{-i\omega t} + c.c.$ ← see bottom of page 3

we seem to have found $\sigma^*_{\alpha\beta}$, such that

$$\sigma_{\alpha\beta} = \frac{iN^2\omega}{\hbar} \sum_n \left[-\frac{\langle 0 | \hat{R}_\alpha | n \rangle \langle n | \hat{R}_\beta | 0 \rangle}{\omega + \omega_{n0} + i0^+} + \frac{\langle n | R_\alpha | 0 \rangle \langle 0 | R_\beta | n \rangle}{\omega - \omega_{n0} + i0^+} \right]$$

Notice that the poles are at $\pm\omega_{n0} - i0^+$, so always in the lower half of the complex plane, and therefore $\sigma_{\alpha\beta}$ is analytic in the upper half of the complex plane.

The denominators $\dfrac{\mp i}{\omega \mp \omega_{no} + i0^+} = \lim_{\varepsilon \to 0^+} \left\{ \dfrac{\mp \varepsilon}{(\omega \mp \omega_{no})^2 + \varepsilon^2} \mp i \dfrac{\omega \pm \omega_{no}}{(\omega \mp \omega_{no})^2 + \varepsilon^2} \right\}$

$$= \mp \pi\, \delta(\omega \pm \omega_{no}) \mp i\, P \frac{1}{\omega \pm \omega_{no}}$$

so that the real part of the conductivity is

$$\mathrm{Re}\,\sigma_{\alpha\beta} = \frac{\pi M^2}{\hbar} \sum_n \omega \Big[- \langle 0|R_\alpha|n\rangle\langle n|R_\beta|0\rangle\, \delta(\omega + \omega_{no})$$
$$+ \langle 0|R_\beta|n\rangle\langle n|R_\alpha|0\rangle\, \delta(\omega - \omega_{no}) \Big]$$

So $\mathrm{Re}\,\sigma_{\alpha\beta}(-\omega) = \mathrm{Re}\,\sigma_{\beta\alpha}(\omega)$

however $\mathrm{Im}\,\sigma_{\alpha\beta}(-\omega) = -\mathrm{Im}\,\sigma_{\beta\alpha}(\omega)$

so that $\underline{\sigma_{\alpha\beta}(-\omega) = \sigma_{\beta\alpha}^*(\omega)}$

This tells you that $\sigma_{xx}(\omega)$ is the Fourier transform of a real quantity. It is the current response function.

Sum rule

Typical perturbative response follows sum rules, reflecting conservation laws or thermodynamics of equilibrium.

Here, $S_0 \equiv \frac{1}{\pi} \int d\omega \; \mathrm{Re}\, \sigma_{\alpha\beta}(\omega)$

Applying this to the perturbative $\sigma_{\alpha\beta}$ we found here, S_0 can be shown to be $\boxed{S_0 = \frac{N^2}{\hbar^2} \left\langle \left[\hat{R}_\alpha, \left[\hat{H}, \hat{R}_\beta \right] \right] \right\rangle}$

or, writing this with $[H, X_{cm}] = -\frac{i\hbar}{N} J_x$,

$$S_0 = \frac{N}{i\hbar} \left\langle \left[\hat{R}_\alpha , \hat{J}_\beta \right] \right\rangle$$

This is a powerful relation because it relates the dynamic response $\sigma(\omega)$ to equilibrium evaluation of commutators.

Let's take a few examples of simple systems.

Free particles

$$\hat{H} = \sum_{j}^{N} \frac{1}{2m} \left(p_{xj}^2 + p_{yj}^2 + p_{zj}^2 \right) \underbrace{+ V(\hat{r}_1 \cdots r_N)}$$

where $V(\cdots)$ can include traps or interactions,

$$[\hat{H}, \hat{X}_{cm}] = \frac{1}{2mN} \sum_{j,i} [\hat{p}_{xi}^2, \hat{x}_i] = \frac{i\hbar}{mN} \sum_j \hat{p}_{xj}$$

or $\hat{J}_x = \frac{iN}{\hbar} [\hat{H}, \hat{X}_{cm}] = \sum \frac{\hat{p}_{xj}}{m}$ sum of velocities!

Now $[\hat{Y}_{cm}, [\hat{H}, \hat{X}_{cm}]] = \frac{i\hbar}{mN^2} \sum_{j,i} [\hat{y}_i, \hat{p}_{xj}]$

$$= \frac{\hbar^2}{mN} \delta_{xy}$$

so the f-sum is diagonal —

$$(S_0)_{\alpha\beta} = \frac{2}{\pi} \int_0^\infty d\omega \, \mathrm{Re}\, \sigma_{\alpha\beta}(\omega) = \frac{N}{m} \delta_{\alpha\beta}$$

This is independent of temperature, interaction strength, or trapping potential.

HM

in TB limit,

$$(S_0)_{xx} = \frac{N}{i\hbar}\left\langle \left[\hat{R}_x , \hat{J}_x \right] \right\rangle \quad , \quad J_x = \frac{-ita_L}{\hbar} \sum_j \left(\hat{c}_j^+ \hat{c}_{j+1} - h.c. \right)$$

$$= -\frac{ta_L}{\hbar^2} \sum_\ell \sum_j \left\langle \left[x_\ell \hat{n}_\ell , \hat{c}_j^+ \hat{c}_{j+1} - \hat{c}_{j+1}^+ \hat{c}_j \right] \right\rangle$$

$$= \frac{a_L^2}{\hbar} t \underbrace{\sum_j \left\langle \hat{c}_j^+ \hat{c}_{j+1} + h.c. \right\rangle}_{\text{but this is the original } \hat{H}_{0x}}$$

So that

$$(S_0)_{xx} = \frac{-a_L^2}{\hbar^2} \langle \hat{H}_{0x} \rangle$$

where, for an isotropic lattice, $\langle \hat{H}_{0x} \rangle$ is $1/d$ of the total kinetic energy, in d dimensions.

$$\rightarrow \quad (S_0)_{xx} = -\frac{a_L^2}{\hbar^2} \frac{E_K}{d}$$

One then interprets the sum rule as the kinetic energy of the gas, times constants.

Both this and N/m are units $1/\text{mass}$, & extensive. The connection between them is more clear if we calculate the thermally averaged effective mass, $\left\langle \frac{1}{m^*} \right\rangle = \int d^3q \, f(q) \frac{1}{m^*(q)}$.

$\longrightarrow$

Simplest version of this average is for 1D, TB HM:

$$\frac{1}{m^*(q)} = \frac{a_L^2}{\hbar^2} \sum 2 t_r r^2 \cos rq$$

$$\left\langle \frac{1}{m^*} \right\rangle = \frac{a_L^2}{\hbar^2} \sum r^2 \langle 2 t_r \cos rq \rangle$$

Hm, only $r=1$ ⟶ this is only case where $E_K = .. S_0$

then

$$\left\langle \frac{1}{m^*} \right\rangle = \frac{a_L^2}{\hbar^2} \underbrace{\langle 2t \cos q \rangle}_{-\langle \hat{H}_{0x} \rangle \text{ for single particle}}$$

& thus $\boxed{S_0 = N \left\langle \frac{1}{m^*} \right\rangle}$

This turns out to be more general — i.e., even for HM with next-nearest coupling etc, than $S_0 = .. E_K$.
(Stronger than the assumptions of the derivation shown here.)