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RESEARCH WORKSHOP ON CONDENSED MATTER PHYSICS
(21 June - 3 September 1993)

WORKING PARTY ON SMALL SEMICONDUCTOR STRUCTURES
(2 - 13 August 1993)

FREQUENCY DEPENDENT CURRENT PARTITION

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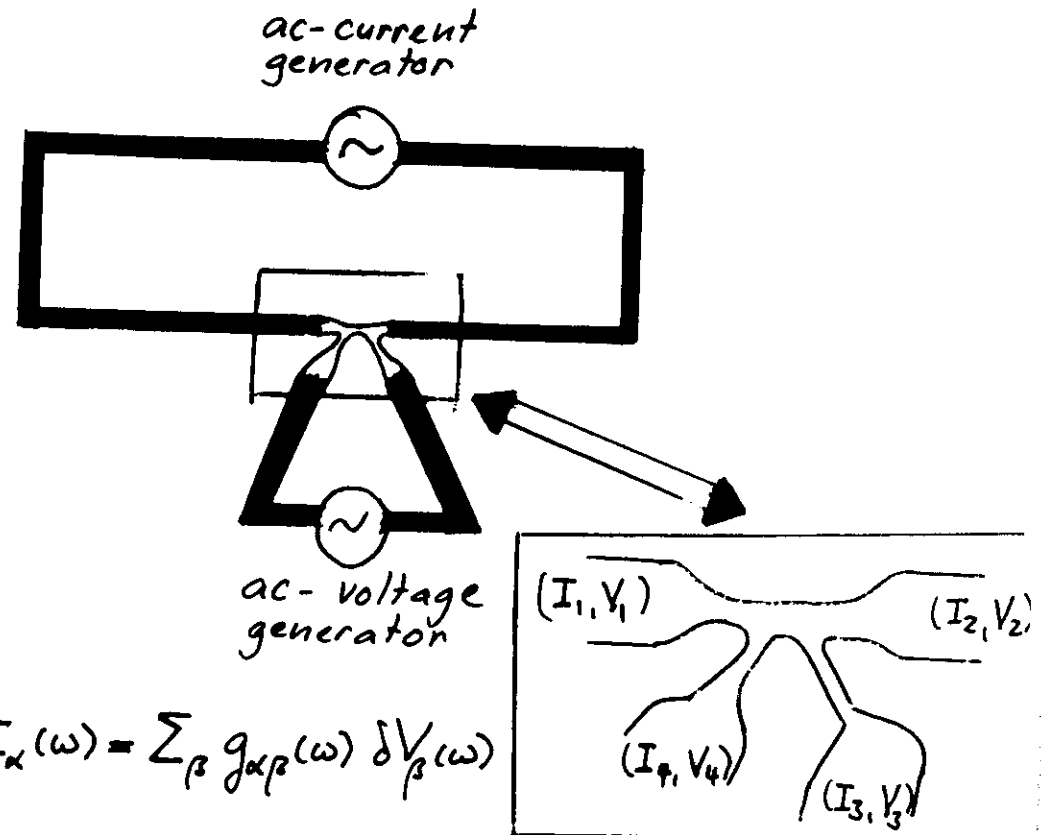
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Frequency-Dependent Current-Partition in Multiprobe Conductors

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AC-Response of Mesoscopic Conductor Embedded in an External Circuit



$$\delta I_\alpha(\omega) = \sum_\beta g_{\alpha\beta}(\omega) \delta V_\beta(\omega)$$

Contrast with formal linear response:

$$H = H_0 + H_1$$

$$H_1 = - \int d^3r \, \rho(\mathbf{r}, t) U_{\text{ext}}(\mathbf{r}, t) + \int d^3r \, \vec{j}(\mathbf{r}, t) \cdot \vec{A}_{\text{ext}}(\mathbf{r}, t)$$

Current Conservation

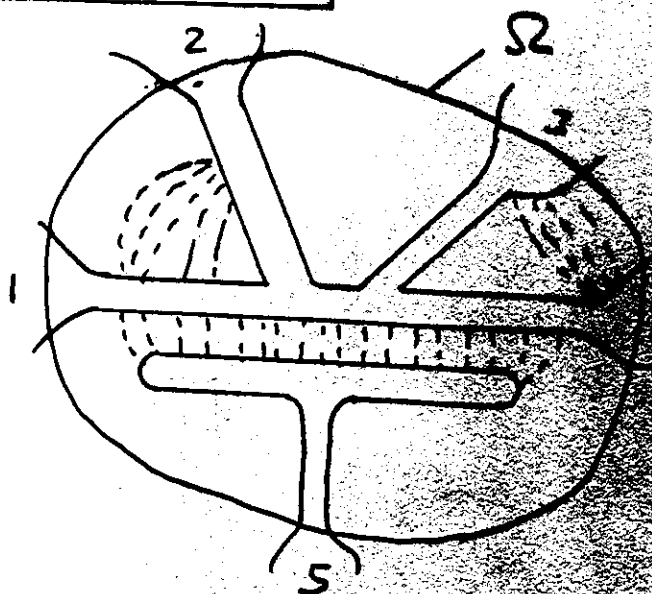
$$\partial \rho / \partial t + \operatorname{div} \vec{j} = 0$$

$$\operatorname{div} \vec{E} = \frac{1}{\epsilon} \rho, \quad \vec{D} = \epsilon \vec{E}$$

$$\operatorname{div} \left(\frac{\partial \vec{D}}{\partial t} + \vec{j} \right) = 0$$

Assume that external circuit can be described in quasi-stationary limit $\leftrightarrow \partial \vec{D} / \partial t \approx 0$ in external circuit. $\Rightarrow$

$$\sum_{\alpha} \delta I_{\alpha}(\omega) = 0$$



$$\int_{\Omega} d\vec{r} \rho(\omega, \vec{r}) =$$

Program

$$d\rho_{\alpha}(\omega)$$



$$\delta I_{\alpha}(\omega) = Z_{\alpha} g_{\alpha}^e(\omega) (d\rho_{\alpha}(\omega)/e)$$

$$dn_{\alpha}(\omega, \vec{r})$$



$$d\mu_{\alpha}(\omega, \vec{r})$$

$$dn_{\alpha}^i(\omega, \vec{r})$$

} self-consistent internal potential



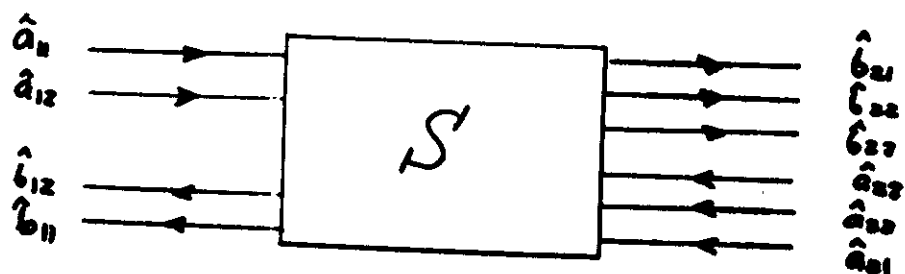
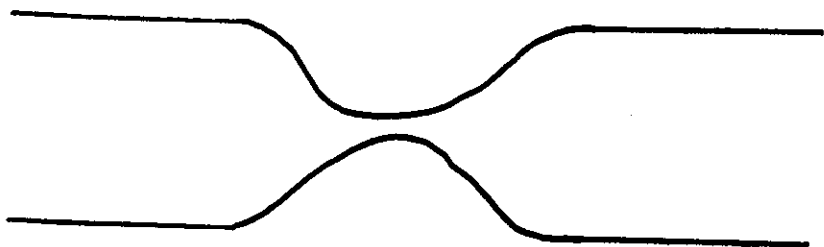
$$\delta I_{\alpha}(\omega) = Z_{\alpha} g_{\alpha}^i(\omega) (d\rho_{\alpha}(\omega)/e)$$



$$\delta I_{\alpha}(\omega) = Z_{\alpha} (g_{\alpha}^e(\omega) + g_{\alpha}^i(\omega)) (d\rho_{\alpha}(\omega)/e)$$

Response to External Potentials

Current operator



$$\hat{\Psi}(r,t) = \hat{\Psi}_+(r,t) + \hat{\Psi}_-(r,t) \rightarrow \hat{j}(r,t) \quad \left(\frac{v_F}{2}, \frac{\lambda_F}{2}\right)$$

$$\hat{I}_\alpha(t) = \hat{I}_{\alpha+}(t) - \hat{I}_{\alpha-}(t) =$$

$$= \frac{e}{h} \int dE dE' (\hat{a}_\alpha^\dagger(E) \hat{a}_\alpha(E') - \hat{b}_\alpha^\dagger(E) \hat{b}_\alpha(E')) e^{i(E-E')t/\hbar}$$

"current amplitude": $\left(\frac{e}{h}\right)^{1/2} \hat{a}(E) dE$

Current Response to Oscillating External Potentials

$$\mu_\alpha(t) = \mu_0 + \delta\mu_\alpha \cos(\omega t)$$

→

$$\hat{a}'_{\alpha m}(E,t) = \hat{a}_{\alpha m}(E) e^{-i(E_{\alpha m} - \mu_0)t/\hbar - i\varphi(t)}$$

$$\varphi(t) = \int dt' \delta\mu_\alpha \cos(\omega t') = (\delta\mu_\alpha / \hbar \omega) \sin(\omega t)$$

⇒

$$\hat{a}'_{\alpha m}(E) = \hat{a}_{\alpha m}(E) + \hat{a}_{\alpha m}(E + \hbar\omega) (\delta\mu_\alpha / 2\hbar\omega) - \hat{a}_{\alpha m}(E - \hbar\omega) (\delta\mu_\alpha / 2\hbar\omega) + \dots$$

$$\hat{b}_\alpha(E) = \sum_\beta S_{\alpha\beta}(E) \hat{a}_\beta(E)$$

⇒

$$g_{\mu\mu}^e(\omega) = \frac{e^2}{h} \int dE \text{Tr} \left[\hat{S}_\mu(E) \hat{S}_\mu^\dagger(E) - \hat{S}_\mu^\dagger(E) \hat{S}_\mu(E + \hbar\omega) \right] \frac{f(E) - f(E + \hbar\omega)}{\hbar\omega}$$

Low-frequency expansion

$$f_{\alpha\beta}^c(\omega) = \frac{e^2}{h} \int dE \operatorname{Tr} [f_{\alpha}(E) S_{\alpha\beta} - S_{\alpha\beta}^{\dagger}(E) f_{\beta}(E + \hbar\omega)] - \frac{f_{\beta}(E) - f_{\beta}(E + \hbar\omega)}{\hbar\omega}$$

$$g_{\alpha\alpha}(0) = \frac{e^2}{h} \int dE (-df/dE) R_{\alpha\alpha}(E)$$

$$g_{\alpha\beta}(0) = -\frac{e^2}{h} \int dE (-df/dE) T_{\alpha\beta}(E)$$

$$\sum_{\alpha} g_{\alpha\beta}(0) = \sum_{\beta} g_{\alpha\beta}(0) = 0$$

First order in ω

$$g_{\alpha\beta}(\omega) = g_{\alpha\beta}(0) - i\omega e^2 \int dE (-df/dE) (dN_{\alpha\beta}/dE)$$

$$\frac{dN_{\alpha\beta}}{dE} = \frac{1}{4\pi i} \operatorname{Tr} \left[S_{\alpha\beta}^{\dagger}(E) \frac{\partial S_{\alpha\beta}(E)}{\partial E} - \frac{\partial S_{\alpha\beta}^{\dagger}(E)}{\partial E} S_{\alpha\beta}(E) \right]$$

Emittance of α

$$\sum_{\beta} g_{\alpha\beta}(\omega) = -i\omega e^2 \int dE (-df/dE) (dN_{\alpha}/dE) \neq 0$$

$$dN_{\alpha}/dE = \sum_{\beta} (dN_{\alpha\beta}/dE) \quad \text{Injectance of } \beta$$

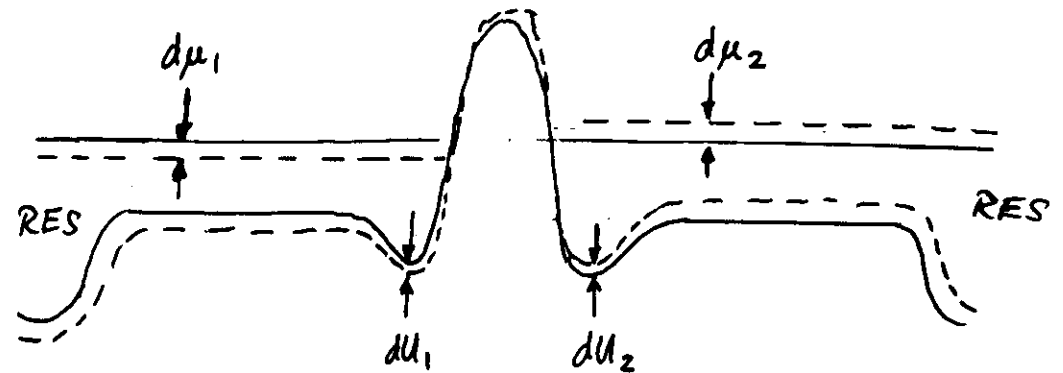
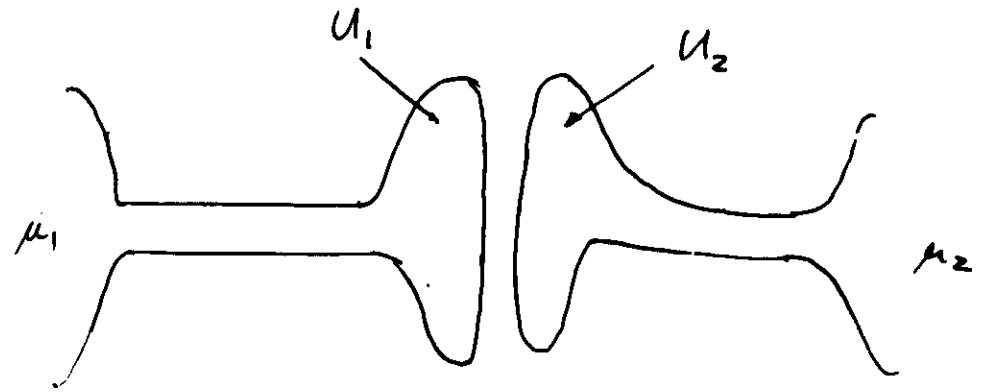
$$\sum_{\alpha} g_{\alpha\beta}(\omega) = -i\omega e^2 \int dE (-df/dE) (d\tilde{N}_{\beta}/dE) \neq 0$$

$$d\tilde{N}_{\beta}/dE = \sum_{\alpha} (dN_{\alpha\beta}/dE)$$

$$B=0 \Rightarrow dN_{\alpha}/dE = d\tilde{N}_{\beta}/dE$$

†

Mesoscopic Capacitor



$$dQ_1 = e (dN_1/dE) (d\mu_1 - e dU_1) = C_e (dU_1 - dU_2)$$

$$dQ_2 = e (dN_2/dE) (d\mu_2 - e dU_2) = C_e (dU_2 - dU_1)$$

$$dQ = dQ_1 = -dQ_2 = C_{\mu} (d\mu_1 - d\mu_2)/e \Rightarrow$$

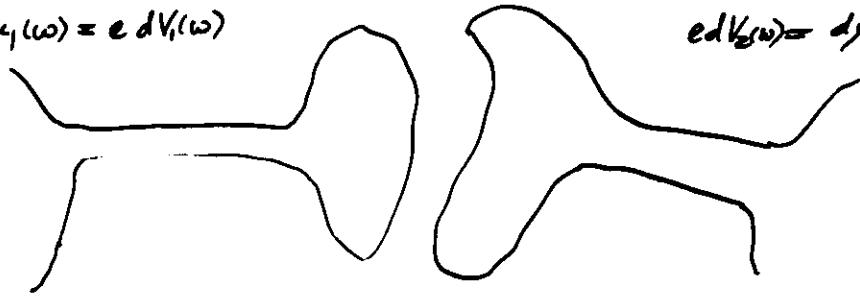
$$\frac{1}{C_{\mu}} = \frac{d\mu}{edQ} = \frac{1}{C_e} + \frac{1}{e^2} \frac{dN_1/dE}{dE} + \frac{1}{e^2} \frac{dN_2/dE}{dE}$$

electro-chemical capacitance

Admittance of a Mesoscopic Capacitor

$$d\mu_1(\omega) = e dV_1(\omega)$$

$$e dV_2(\omega) = d\mu_2(\omega)$$



$$dI_1(\omega) = g_{11}^e(\omega) dV_1(\omega) + g_{11}^i(\omega) dU_1(\omega) = -i\omega C_e (dU_1(\omega) - dU_2(\omega))$$

$$dI_2(\omega) = g_{22}^e(\omega) dV_2(\omega) + g_{22}^i(\omega) dU_2(\omega) = -i\omega C_e (dU_2(\omega) - dU_1(\omega))$$

Invariance against global potential shift $\Rightarrow$

$$g_{11}^i(\omega) = -g_{11}^e(\omega) ; \quad g_{22}^i(\omega) = -g_{22}^e(\omega)$$

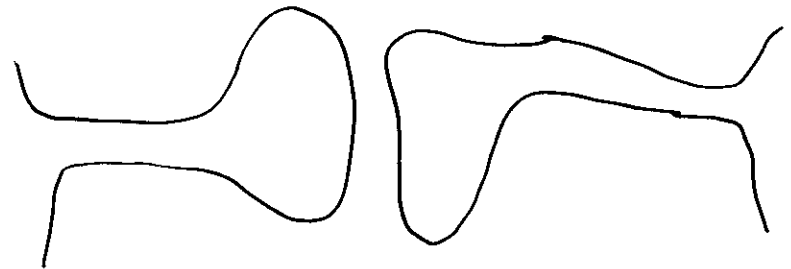
$$\Rightarrow dI(\omega) = g^I(\omega) (dV_1(\omega) - dV_2(\omega))$$

$$g^I(\omega) = -i\omega C_\mu + \omega^2 C_\mu^2 R_q + O(\omega^3)$$

$$R_q = R_1 + R_2 \quad \text{charge relaxation resistance}$$

$$R_q = \frac{h}{2e^2} \frac{\int dE (-df/dE) \text{Tr} [S_{\text{out}}^\dagger(E) dS_{\text{out}}(E)/dE]^2}{(\int dE (-df/dE) \text{Tr} [S_{\text{out}}^\dagger(E) dS_{\text{out}}(E)/dE])^2}$$

Noise Spectrum of a Capacitor



$$g^I(\omega) = -i\omega C_\mu + \omega^2 C_\mu^2 R_q + O(\omega^3)$$

$\langle (\Delta I(\omega))^2 \rangle$ follows from FDT MB PRB45,3807(9)
PRB46,12485(9)

$$I_1 = g_{11}(\omega) (dV_1(\omega) - dU_1(\omega)) + \delta I_1(\omega) = -i\omega C_e (dU_1(\omega) - dU_2(\omega))$$

$$I_2 = g_{22}(\omega) (dV_2(\omega) - dU_2(\omega)) + \delta I_2(\omega) = -i\omega C_e (dU_2(\omega) - dU_1(\omega))$$

zero external impedance $\rightarrow dV_1 = dV_2 = 0 \Rightarrow$

$$\langle (\Delta I(\omega))^2 \rangle = 2 |g^I(\omega)|^2 \left(\frac{g_{11}'(\omega)}{|g_{11}(\omega)|^2} + \frac{g_{22}'(\omega)}{|g_{22}(\omega)|^2} \right) \varepsilon(\frac{1}{2}\omega, kT)$$

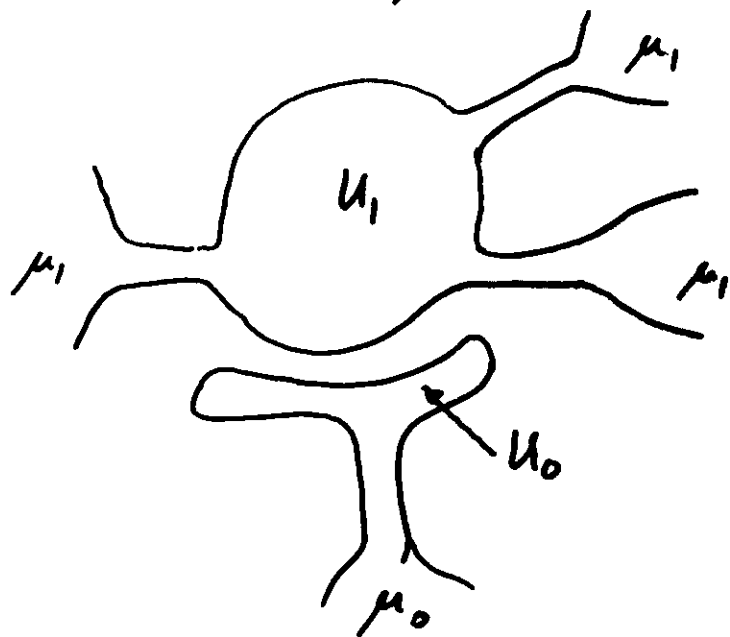
$$= 2 (g^I(\omega))' \varepsilon(\frac{1}{2}\omega, kT)$$

$$= 2kT \omega^2 C_\mu^2 R_q + O(\omega^4)$$

infinite external impedance $\rightarrow dI_1 = dI_2 = 0 \Rightarrow$

$$\langle (\Delta V(\omega))^2 \rangle = 2kT R_q + O(\omega^2)$$

Electro-Chemical Capacitance



$$dQ_1 = e \left(\frac{dN_1}{dE} \right) (d\mu_1 - e dU_1) = C (dU_1 - dU_2)$$

$$dQ_2 = e \left(\frac{dN_0}{dE} \right) (d\mu_0 - e dU_0) = C (dU_2 - dU_1)$$

$$\frac{dN_1}{dE} = \sum_{\alpha} \frac{dN_{\alpha}}{dE} = \sum_{\alpha} \frac{d\tilde{N}_{\alpha}}{dE} = \sum_{\alpha \neq 1} \frac{dN_{\alpha}}{dE}$$

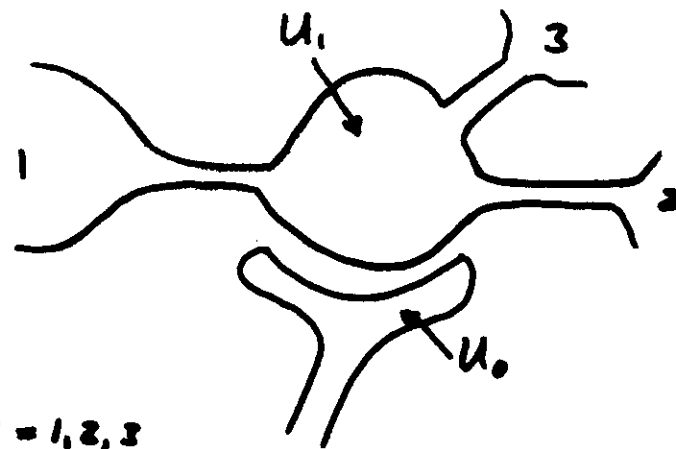
→

$$dQ = dQ_1 = -dQ_2 = C_{\mu} (d\mu_1 - d\mu_2)/e$$

→

$$\boxed{\frac{1}{C_{\mu}} = \frac{1}{C} + \frac{1}{e^2 \frac{dN_0}{dE}} + \frac{1}{e^2 \frac{dN_1}{dE}}}$$

Simple Model with two Internal Voltages



$\alpha = 1, 2, 3$

$$I_{\alpha} = \sum_{\beta} g_{\alpha\beta}^e dV_{\beta} + g_{\alpha 1}^i dU_1$$

$$I_0 = g_{00}^e dV_0 + g_{00}^i dU_0$$

$$\sum_{\alpha} I_{\alpha} = -i\omega C (dU_1 - dU_0)$$

$$I_0 = -i\omega C (dU_0 - dU_1)$$

Invariance against global potential shift

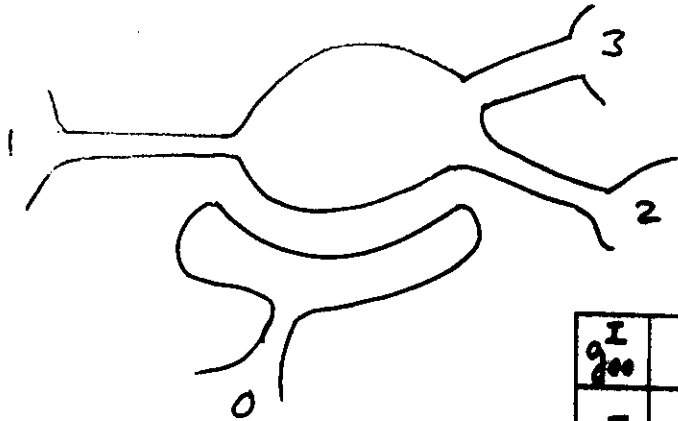
$$(dV_{\alpha}, dU_0, dU_1) \leftrightarrow (dV_{\alpha} - dU_1, dU_0 - dU_1, 0) \leftrightarrow$$

$$(dV_{\alpha} - dU_0, 0, dU_1 - dU_0)$$

⇒

$$g_{00}^i = -g_{00}^e, \quad g_{\alpha 1}^i = -\sum_{\beta} g_{\alpha\beta}^e$$

Simple Model: Lowest Order Admittance Tensor



g_{00}^I	g_{01}^I	g_{02}^I	g_{03}^I
g_{10}^I	g_{11}^I	g_{12}^I	g_{13}^I
g_{20}^I	g_{21}^I	g_{22}^I	g_{23}^I
g_{30}^I	g_{31}^I	g_{32}^I	g_{33}^I

$$\frac{1}{C_\mu} = \frac{1}{C} + \frac{1}{e^2(dN_0/dE)} + \frac{1}{e^2(dN_1/dE)}$$

$$\frac{1}{C_0} = \frac{1}{C} + \frac{1}{e^2(dN_0/dE)}$$

$$g_{00}^I(\omega) = -i\omega C_\mu$$

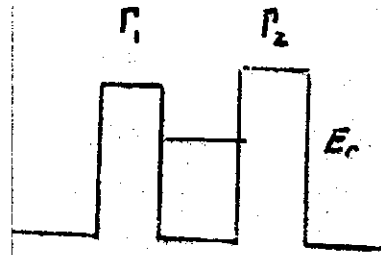
$$g_{0\alpha}^I(\omega) = i\omega C_\mu \frac{d\tilde{N}_\alpha/dE}{dN_1/dE}$$

$$g_{\alpha 0}^I(\omega) = i\omega C_\mu \frac{dN_\alpha/dE}{dN_1/dE}$$

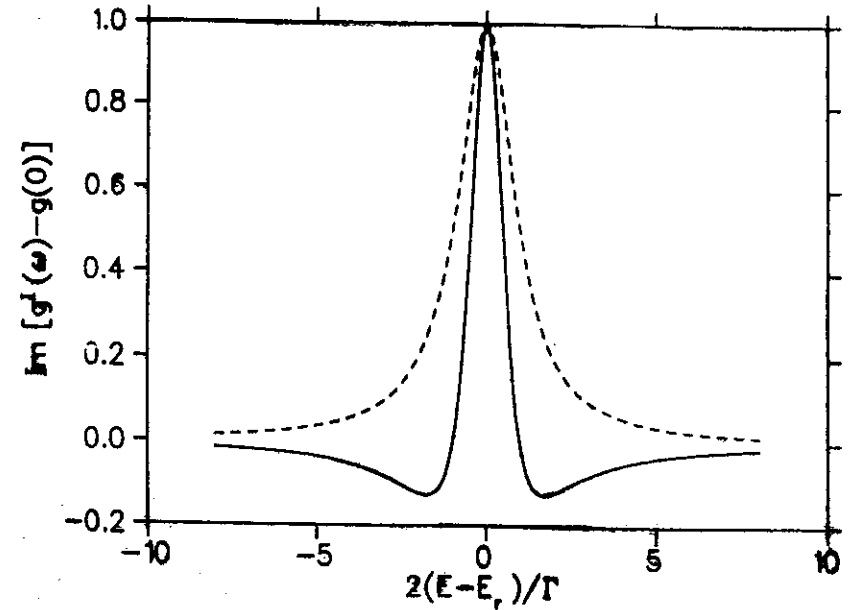
$$g_{\alpha\beta}^I(\omega) = g_{\alpha\beta}(0) - i\omega e^2 dN_{\alpha\beta}/dE + i\omega e^2 \frac{C_\mu (dN_\alpha/dE)(d\tilde{N}_\beta/dE)}{C_0 (dN_1/dE)}$$

$$\frac{C_\mu - C_0}{C_0} = -\frac{C_\mu}{e^2(dN_1/dE)}$$

Two simple limits: $N \rightarrow \frac{\omega}{E}$



$$S_{\alpha\beta}(E) = \left(\delta_{\alpha\beta} - \frac{i \Gamma_\alpha^{1/2} \Gamma_\beta^{1/2}}{E - E_r - c\mathcal{U} + i \frac{\Gamma}{2}} \right) e^{i(\delta_\alpha + \delta_\beta)}$$

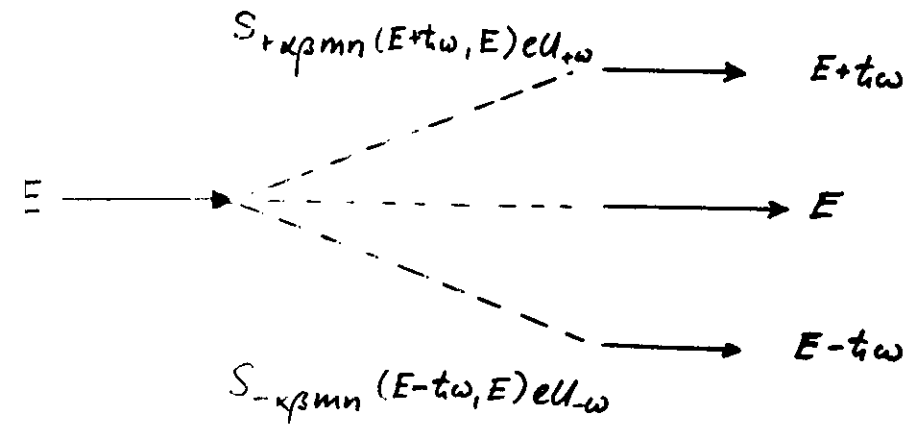


$$g^I(\omega) = g(0) + i \left(\frac{\omega E}{2\Gamma} \right) \left(\frac{\Gamma E}{|\Delta|^2} \right) \frac{(\Gamma^2/2 - |\Delta|^2)}{|\Delta|^2}$$

$$|\Delta|^2 = (E - E_r)^2 + \Gamma^2/4$$

Current Response to an Arbitrary Internal Potential

$$U(r, t) = V(r) (U_{+\omega} e^{-i\omega t} + U_{-\omega} e^{i\omega t})$$



$$\begin{aligned} \hat{a}_{\alpha n}(E) = \sum_{\beta n} & (S_{+\alpha\beta mn}(E) \hat{a}_{\beta n}(E) \\ & + S_{-\alpha\beta mn}(E, E + \hbar\omega) eU_{-\omega} \hat{a}_{\beta n}(E + \hbar\omega) \\ & + S_{+\alpha\beta mn}(E, E - \hbar\omega) eU_{+\omega} \hat{a}_{\beta n}(E - \hbar\omega) \\ & + \dots) \end{aligned}$$

$$\begin{aligned} g_{\alpha}^i(\omega) &= -\frac{e^2}{\hbar} \sum_{\beta} \int dE \\ & [S_{+\alpha\beta}^{\dagger}(E) S_{+\alpha\beta}(E + \hbar\omega, E) f(E) + S_{+\alpha\beta}^{\dagger}(E, E + \hbar\omega) S_{+\alpha\beta}(E + \hbar\omega) f(E + \hbar\omega)] \\ \text{unitarity: } \sum_{\beta} & [S_{+\alpha\beta}^{\dagger}(E, E + \hbar\omega) S_{+\alpha\beta}(E + \hbar\omega) + S_{+\alpha\beta}^{\dagger}(E) S_{+\alpha\beta}(E + \hbar\omega, E)] = 0 \\ g_{\alpha}^i(\omega) &= -\frac{e^2}{\hbar} \sum_{\beta} \int dE \text{Tr} [S_{+\alpha\beta}^{\dagger}(E) S_{+\alpha\beta}(E + \hbar\omega, E)] (f(E) - f(E + \hbar\omega)) \end{aligned}$$

Current Response to Slowly Changing Internal Potential

$$g_{\alpha}^i(\omega) = -\frac{e^2}{\hbar} \sum_{\beta} \int dE \text{Tr} [S_{+\alpha\beta}^{\dagger}(E) S_{+\alpha\beta}(E + \hbar\omega, E)] (f(E) - f(E + \hbar\omega))$$

$$\omega \rightarrow 0 \quad ?$$

$$S(E, U(r)) \rightarrow S(E, U(r, t))$$

$$U(r, t) = V(r) (U_{+\omega} e^{-i\omega t} + U_{-\omega} e^{i\omega t})$$

$$\lim_{\omega \rightarrow 0} S_{+\alpha\beta}(E + \hbar\omega, E) = \int d^3r \frac{\partial S_{\alpha\beta}(E)}{\partial U(r)} V(r)$$

$$g_{\alpha}^i(\omega) = -ie^2\omega \int d^3r \frac{dn(\omega, r)}{dE} V(r)$$

$$\frac{dn(\omega, r)}{dE} = -\frac{1}{4\pi i} \int dE \left(-\frac{d}{dE}\right) \sum_{\beta} \text{Tr} \left[S_{+\alpha\beta}^{\dagger}(E) \frac{\partial S_{\alpha\beta}(E)}{\partial U(r)} - \left(\frac{\partial S_{+\alpha\beta}^{\dagger}(E)}{\partial U(r)}\right) S_{+\alpha\beta}(E) \right]$$

integrated emissivity modulated by internal potential

Internal Potential from Charge Neutrality

Charge Neutrality Condition

$$\frac{dn(r,\beta)}{dE} \mu_\beta + \left(\frac{\delta n(r)}{\delta \psi(r)} \right) \psi(r) = 0$$

Screening by all locally available charges

$$\frac{\delta n(r)}{e \delta \psi(r)} = - \sum_\alpha \frac{dn(\alpha, r)}{dE} = - \sum_\alpha \frac{dn(r, \alpha)}{dE} = - \frac{dn_{tot}(r)}{dE}$$

$\Rightarrow$

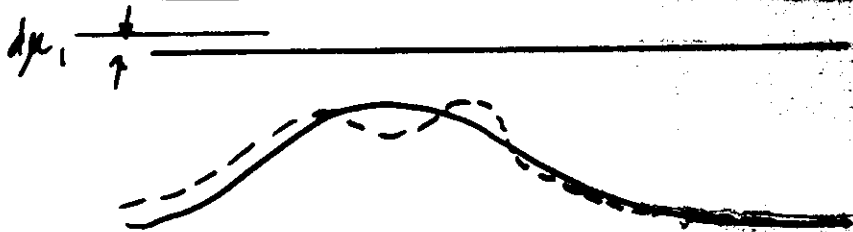
$$\psi(r) = \frac{dE}{dn(r)} \frac{dn(r,\beta)}{dE} d\mu_\beta$$

$\Rightarrow$

$$\begin{aligned} g_\alpha^i(\omega) \psi_{\beta+\omega} &= ie^2 \omega \int d^3r \frac{dn(\alpha, r)}{dE} \psi_\beta(r) \psi_{\beta+\omega} \\ &= ie^2 \omega \int d^3r \frac{dn(\alpha, r)}{dE} \frac{dE}{dn(r)} \frac{dn(r, \beta)}{dE} \delta \mu_\beta(\omega) \end{aligned}$$

$\Rightarrow$

$$g_{\alpha\beta}^i(\omega) = ie^2 \omega \int d^3r \frac{dn(\alpha, r)}{dE} \frac{dE}{dn(r)} \frac{dn(r, \beta)}{dE}$$



Admittance of a charge neutral conductor

● charge neutrality

$$g_{\alpha\beta}^e(\omega) = g_{\alpha\beta}(0) - i\omega e^2 (dN_{\alpha\beta}/dE)$$

$$g_{\alpha\beta}^i(\omega) = i\omega e^2 \int d^3r \frac{\delta n(\alpha, r)}{\delta n(r)} \frac{dn(r, \beta)}{dE}$$

$$g_{\alpha\beta}^I(\omega) = g_{\alpha\beta}^e(\omega) + g_{\alpha\beta}^i(\omega)$$

$$g_{\alpha\beta}^I(\omega) = g_{\alpha\beta}(0) - i\omega e^2 \left[\frac{dN_{\alpha\beta}}{dE} - \int d^3r \frac{\delta n(\alpha, r)}{\delta n(r)} \frac{dn(r, \beta)}{dE} \right]$$

$$\begin{aligned} \delta n(r) = \sum_\alpha \delta n(\alpha, r) &\Rightarrow \sum_\alpha g_{\alpha\beta}^I(\omega) = 0 \\ \sum_\beta g_{\alpha\beta}^I(\omega) &= 0 \end{aligned}$$

Compare with simple model: ($C \rightarrow 0$)

$$g_{\alpha\beta}^I(\omega) = g_{\alpha\beta}(0) - i\omega e^2 \left[\frac{dN_{\alpha\beta}}{dE} - \frac{(dN_\alpha/dE)(dN_\beta/dE)}{(dN/dE)} \right]$$

Long range non-local screening

$$g_{\alpha\beta}^I(\omega) = g_{\alpha\beta}(0) - i\omega e^2 \left[\frac{dN_{\alpha\beta}}{dE} - \int d^3r d^3r' \frac{dn(\alpha, r)}{dE} g(r, r') \frac{dn(r', \beta)}{dE} \right]$$

summary

- ▷ Current Conservation
- ▷ Electro-chemical capacitance
- ▷ Response to external potentials
Response to internal potentials
- ▷ Determine $U(r,t)$ self-consistently

References

- Büttiker, Prêtre, Thomas, PRL 70, 615 (1993)
Büttiker, Thomas, Prêtre, Phys. Lett. A (to appear)
Büttiker, Thomas, Prêtre, preprint on frequency
dependent current partition (write to M.B.)

