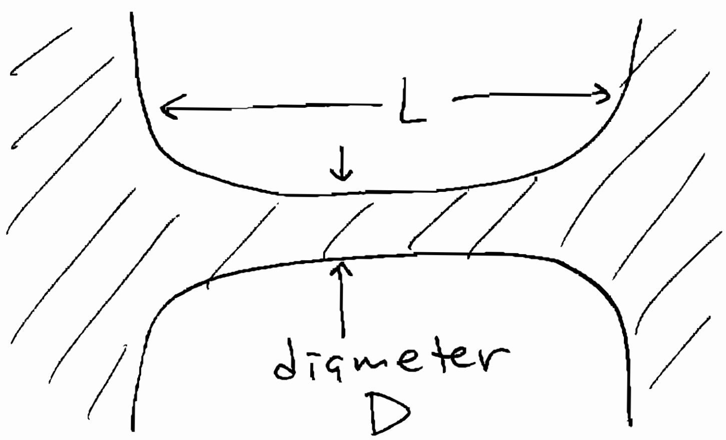
Phys 460/560 Lecture 6

Metallic Nanocohesion

Consider a straight nanowire of metal connecting two electrodes:

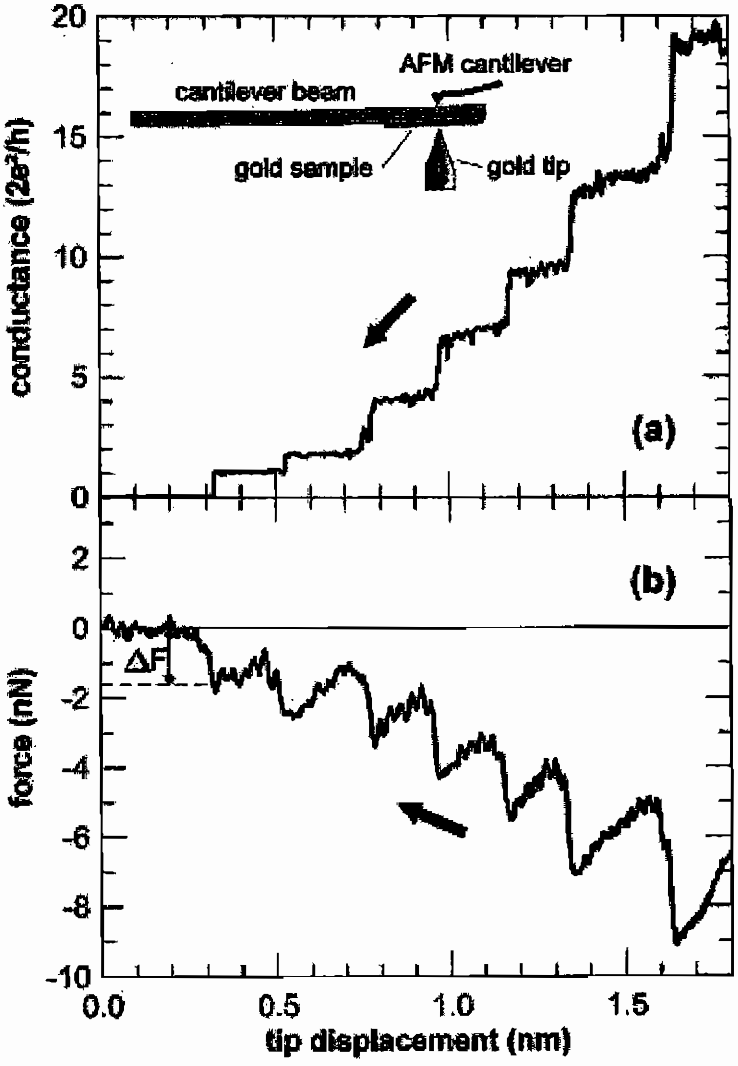


Open system: Grand canonical ensemble

$$\Omega = E - TS - \mu N$$

$T \to 0$: $\Omega = E - \varepsilon_F N$

Experiment with a Gold Nanocontact



$$\Omega_{T=0} = \int_0^{\varepsilon_F} d\varepsilon \left(\varepsilon - \varepsilon_F \right) D(\varepsilon)$$

$D(\varepsilon)$ = density of states

From lecture 14:

$$D(\varepsilon) = L \sum_\nu \frac{4}{h V_\nu}$$

($4 = 2$ (spin) $\times\ 2$ (left and right movers))

$$V_\nu = \sqrt{\frac{2}{M} \left(E - \varepsilon_\nu \right)}$$

Square cross section

$$\varepsilon_\nu = \varepsilon_{nm} = \frac{\hbar^2 \pi^2}{2 M D^2} \left(n^2 + m^2 \right)$$

$$D(\varepsilon) = \frac{4L}{h} \sum_{nm}{}' \frac{1}{\sqrt{\frac{2}{m}(\varepsilon - \varepsilon_{nm})}}$$

(sum only over modes with $\varepsilon > \varepsilon_{nm}$)

$$\Omega = \int_0^{\varepsilon_F} d\varepsilon \, (\varepsilon - \varepsilon_F) \, D(\varepsilon)$$

$$= \frac{4L}{h}\sqrt{\frac{m}{2}} \sum_\nu \int_{\varepsilon_\nu}^{\varepsilon_F} d\varepsilon \, \frac{\varepsilon - \varepsilon_F}{\sqrt{\varepsilon - \varepsilon_\nu}}$$

(integrating by parts)

$$\Omega = -\frac{8}{3}\frac{2L}{h}\sqrt{\frac{m}{2}} \sum_\nu (\varepsilon_F - \varepsilon_\nu)^{3/2}$$

$$\boxed{\Omega = -\frac{8}{3}\frac{\varepsilon_F}{\lambda_F} L \sum_\nu \left(1 - \frac{\varepsilon_\nu}{\varepsilon_F}\right)^{3/2}}$$

When the wire is elongated, the total volume remains more or less constant:

$$V = AL = \text{const.}$$

$$\frac{\varepsilon_{nm}}{\varepsilon_F} = \frac{\frac{\hbar^2\pi^2}{2MD^2}(n^2+m^2)}{\frac{\hbar^2 k_F^2}{2M}}$$

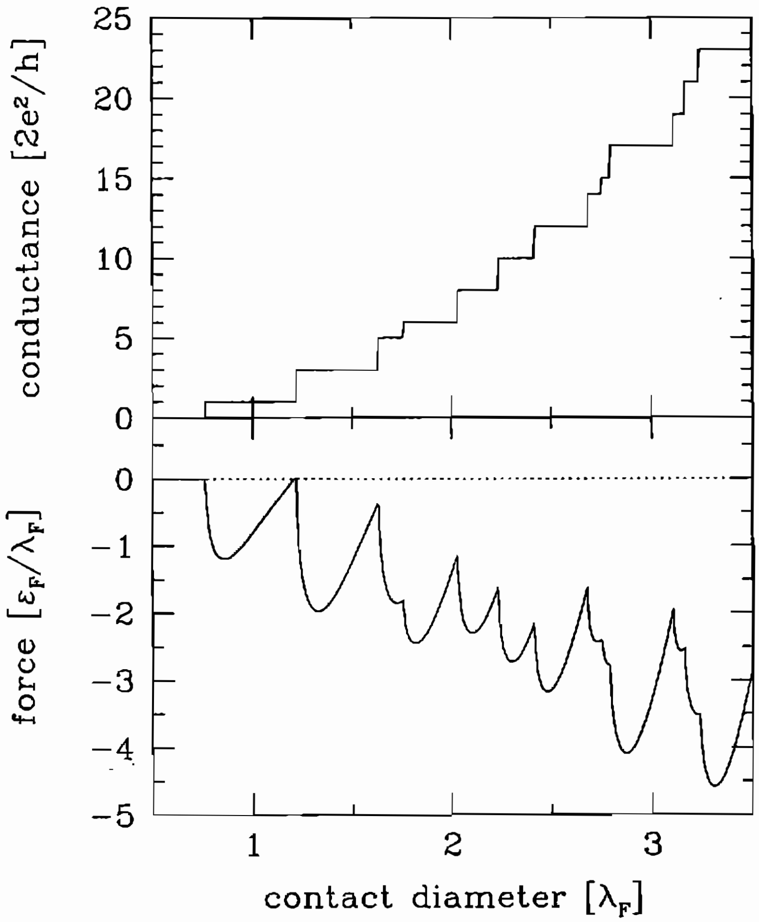
$$= \frac{\pi^2(n^2+m^2)}{k_F^2 A}$$

A = cross-sectional area of wire $= D^2$

Force: $$F = -\frac{\partial \Omega}{\partial L}.$$

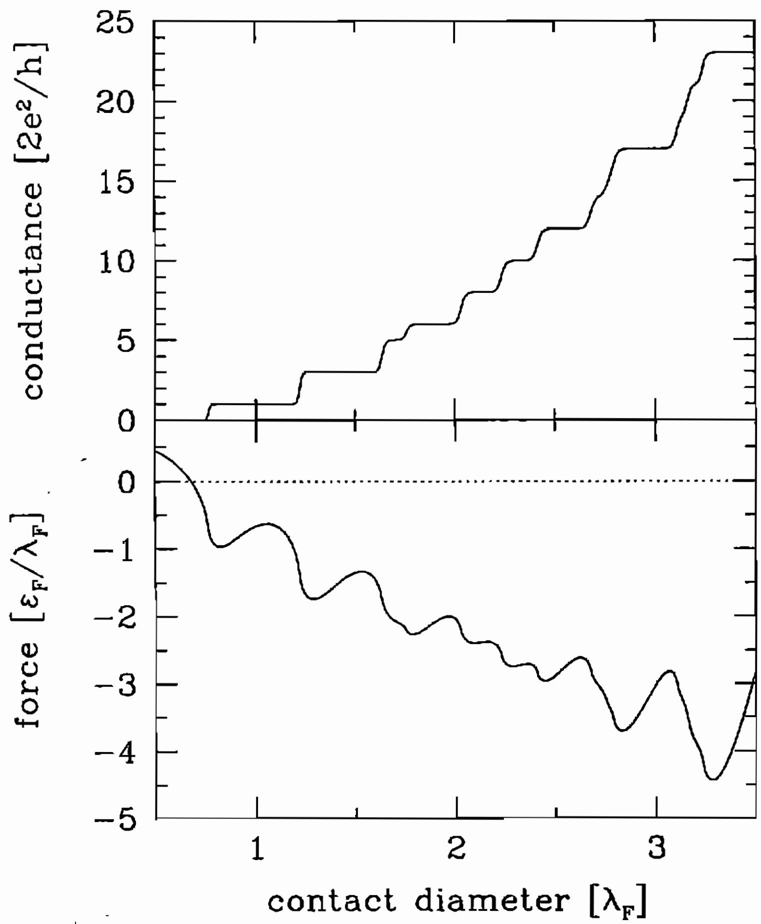
Result for a straight wire

$$F = -\left.\frac{\partial\Omega}{\partial L}\right|_V = \frac{8\varepsilon_F}{3\lambda_F}\sum_{\varepsilon_\nu<\varepsilon_F}\left(1-\frac{5\varepsilon_\nu}{2\varepsilon_F}\right)\left(1-\frac{\varepsilon_\nu}{\varepsilon_F}\right)^{1/2}$$



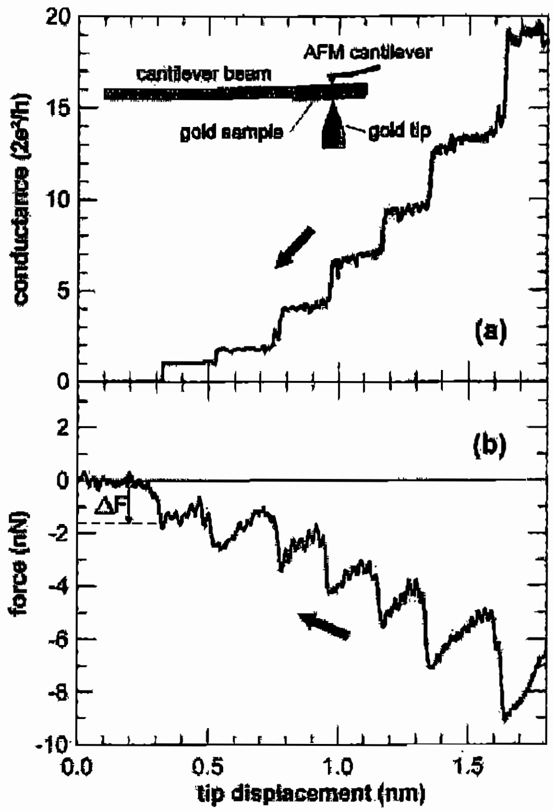
S. Blom et al., PRB **57**, 8830 (1998)

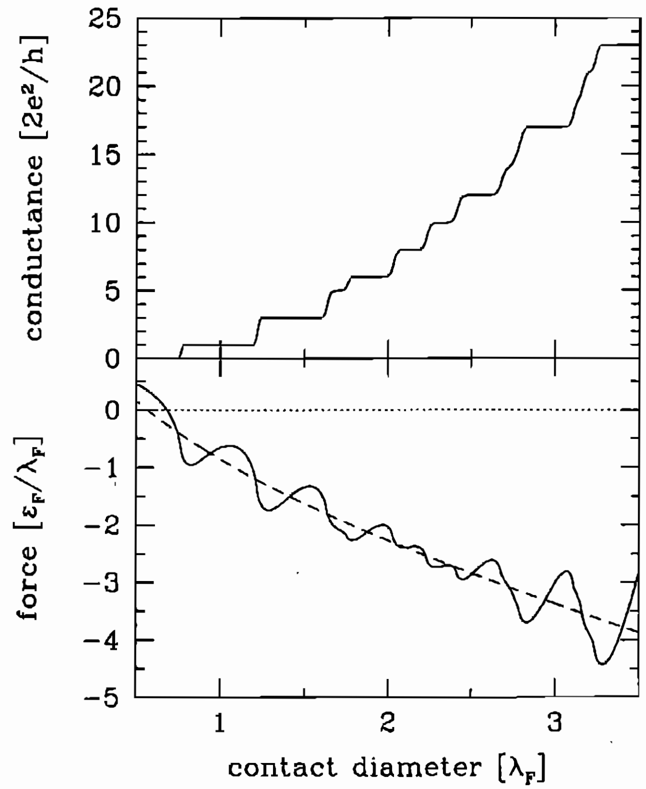
Result for a smooth geometry



Note that $\varepsilon_F/\lambda_F = 1.7\text{nN}$ in gold.

CAS, D. Baeriswyl & J. Bürki, PRL **79**, 2863 (1997)





Left: Experiment with a gold nanocontact. Right: Free-electron calculation. Dashed curve: surface tension approx. Note that $\varepsilon_F/\lambda_F \approx 1.7$nN in gold.

In order to understand the overall behavior of the cohesive force, it is useful to consider how Ω scales with volume, surface area, etc.

$$\Omega = -\frac{8}{3}\frac{\varepsilon_F}{\lambda_F} L \sum_{nm} \left(1 - \frac{\varepsilon_{nm}}{\varepsilon_F}\right)^{3/2}$$

$$= -\frac{8}{3}\frac{\varepsilon_F}{\lambda_F} L \sum_{nm} \left(1 - \left(\frac{\pi n}{k_F D}\right)^2 - \left(\frac{\pi m}{k_F D}\right)^2\right)^{3/2}$$

$$= -\frac{8}{3}\frac{\varepsilon_F}{\lambda_F} L \sum_{n=1}^{\mathrm{int}\left(\sqrt{\left(\frac{k_F D}{\pi}\right)^2 - 1}\right)} \sum_{m=1}^{\mathrm{int}\sqrt{\left(\frac{k_F D}{\pi}\right)^2 - n^2}} \left(1 - \left(\frac{\pi n}{k_F D}\right)^2 - \left(\frac{\pi m}{k_F D}\right)^2\right)^{3/2}$$

Let $n_F = \frac{k_F D}{\pi}$

$$\Omega = -\frac{8}{3}\frac{\varepsilon_F}{\lambda_F} L \sum_{n=1}^{\text{int}\sqrt{n_F^2-1}} \sum_{m=1}^{\text{int}\sqrt{n_F^2-n^2}} \left(1 - \frac{n^2}{n_F^2} - \frac{m^2}{n_F^2}\right)^{3/2}$$

int(x) = largest integer less than or equal to x.

To leading order, we can replace the sums by integrals:

$$\sum_{n=1}^{N} f(n) \simeq \int_0^N f(n)\,dn$$

However, it is useful to keep the first correction terms:

$$\sum_{n=1}^{N} f(n) = \int_0^{N+1} f(n)\,dn - \frac{f(N+1)}{2} - \frac{f(0)}{2} + \cdots$$

Thus

$$\Omega \simeq -\frac{8\mathcal{E}_F}{3\lambda_F} L \int_0^{n_F} dn \int_0^{\sqrt{n_F^2-n^2}} dm \left(1 - \frac{n^2}{n_F^2} - \frac{m^2}{n_F^2}\right)^{3/2}$$

$$+ \frac{4\mathcal{E}_F}{3\lambda_F} L \int_0^{n_F} dn \left(1 - \frac{n^2}{n_F^2}\right)^{3/2}$$

$$+ \frac{4}{3}\frac{\mathcal{E}_F}{\lambda_F} L \int_0^{n_F} dm \left(1 - \frac{m^2}{n_F^2}\right)^{3/2}$$

Let $n = r\cos\theta$, $m = r\sin\theta$

$n^2 + m^2 = r^2$

$dn\,dm \to r\,dr\,d\theta$

$$\Omega \simeq -\frac{8\mathcal{E}_F}{3\lambda_F} L \frac{2\pi}{4} \int_0^{n_F} r\left(1 - \frac{r^2}{n_F^2}\right)^{3/2} dr$$

$$+ \frac{8\mathcal{E}_F}{3\lambda_F} L \int_0^{n_F} dn \left(1 - \frac{n^2}{n_F^2}\right)^{3/2}$$

There are two integrals to evaluate:

$$\int_0^{n_F} r\left(1-\frac{r^2}{n_F^2}\right)^{3/2} dr = \frac{n_F^2}{5} = \frac{k_F^2 A}{5\pi^2}$$

$$\int_0^{n_F} dn\left(1-\frac{n^2}{n_F^2}\right)^{3/2} = n_F \frac{3\pi}{16} = k_F D \frac{3}{16}$$

We find

$$\Omega \simeq -\frac{2\,\varepsilon_F k_F^3}{15\pi^2} V + \frac{\varepsilon_F k_F^2}{16\pi} S,$$

where $V = AL$ = volume

and $S = 4DL$ = surface area.

If the deformation occurs at constant volume, then

$$F = -\frac{\partial \Omega}{\partial L}\bigg|_V \cong -\frac{\varepsilon_F k_F^2}{16\pi}\frac{\partial S}{\partial L}$$

$$S = 4DL \qquad D^2 L = \text{const.} = V$$

$$= 4\sqrt{VL}$$

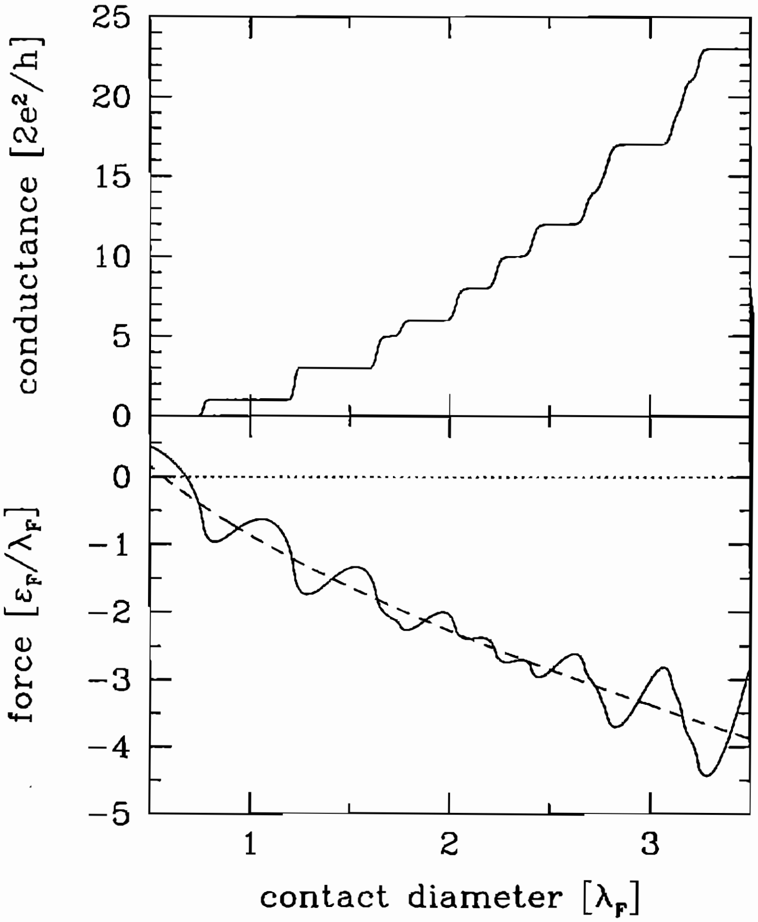
$$\frac{\partial S}{\partial L}\bigg|_V = 2\sqrt{\frac{V}{L}} = 2D$$

$$\boxed{F \simeq -\frac{\varepsilon_F}{\lambda_F}\frac{k_F D}{4} \qquad \text{surface tension force}}$$

On the other hand, the electrical conductance is approximately

$$\boxed{G \simeq \frac{2e^2}{h}\frac{(k_F D)^2}{4\pi} \qquad \text{Sharvin formula}}$$

Cohesive force = surface tension + oscillatory quantum correction



These formulas give the overall trends of force and conductance of a metallic nanowire as a function of its diameter.

To these overall scales are added the quantized plateau structure of the conductance and the quantum oscillations of the force, due to the discrete transverse states in the wire.