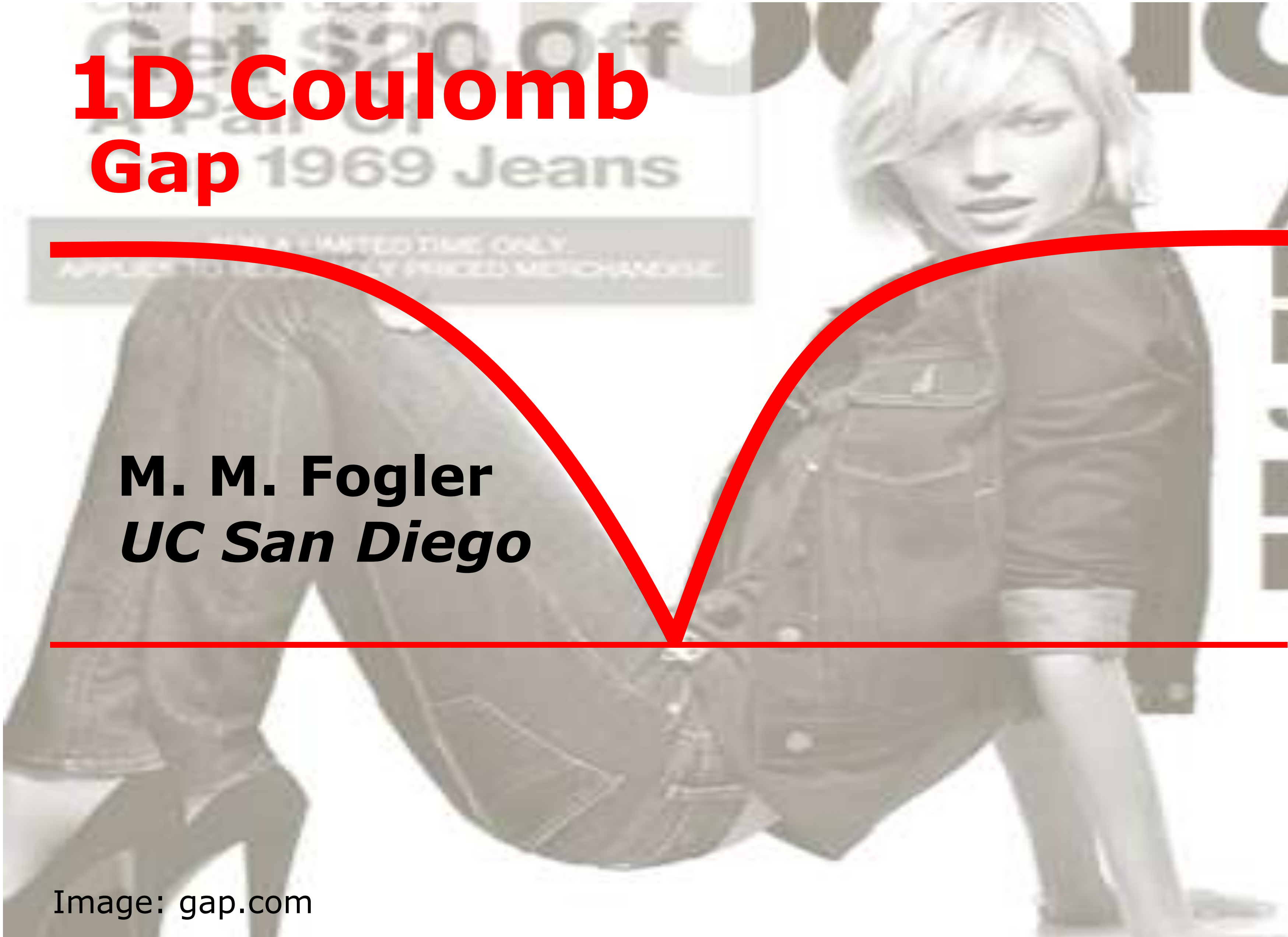
1D Coulomb Gap



M. M. Fogler
UC San Diego

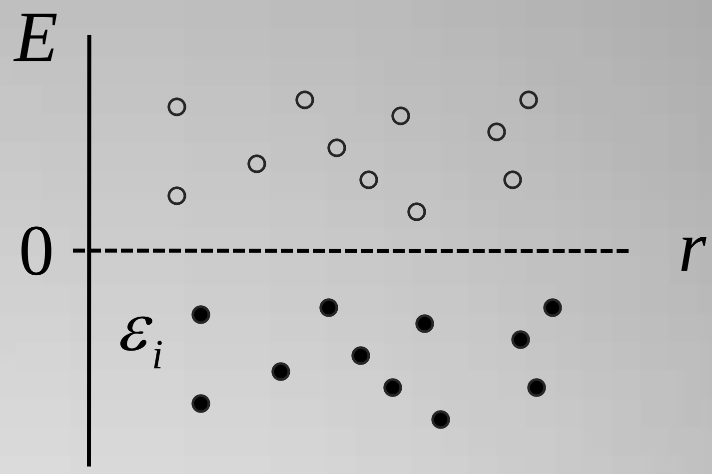
Image: gap.com

What systems have Coulomb gap?

- Disordered systems of localized electrons
- Coulomb interactions remain unscreened

$$\varepsilon_i = \varepsilon_i^0 + \sum_{j \neq i} \frac{e^2}{r_{ij}}$$

- Long-range correlations are important



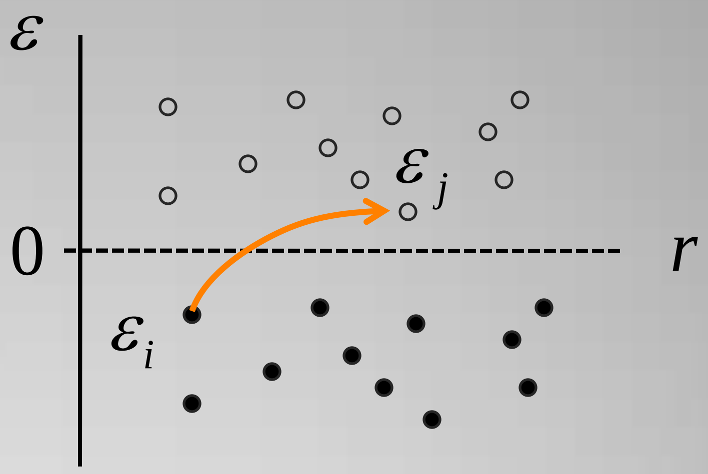
Pollak, 1970
Srinivasan, 1971
Efros & Shklovskii, 1975

Efros-Shklovskii stability criterion

Stability criterion:

$$\varepsilon_j - \varepsilon_i - \frac{e^2}{r_{ij}} \geq 0$$

$$r_{ij} > \frac{e^2}{\varepsilon_j - \varepsilon_i}$$



States near the Fermi level are very *sparse* in space – the density of states is depleted

Coulomb gap in 3, 2, and 1D

Density of states (DOS)

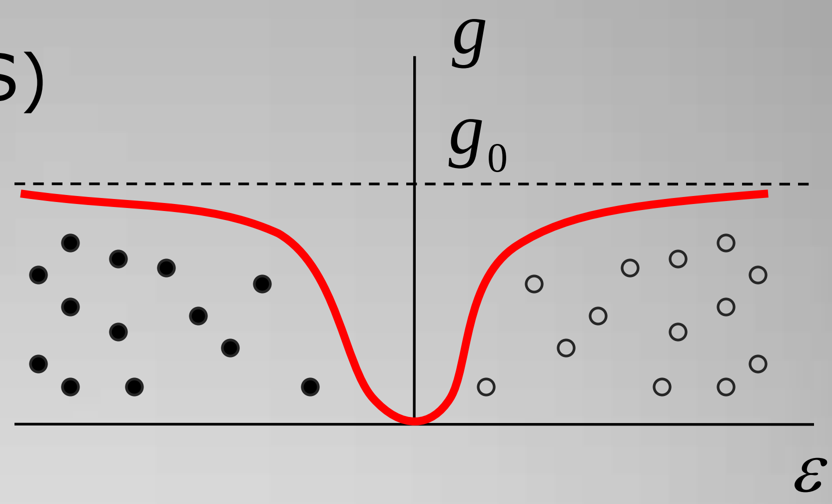
3D: $$g(\varepsilon) \le C_3 e^{-6} \varepsilon^2$$

2D: $$g(\varepsilon) \le C_2 e^{-4} |\varepsilon|$$

Efros & Shklovskii, 1975
Efros, 1976

1D: $$g(\varepsilon) \le \frac{C_1 e^{-2}}{\ln|\varepsilon_* / \varepsilon|}$$

Baranovskii et al, 1980
Raikh & Efros, 1987
Vojta & John, 1993
Johnson & Khmelnitskii, 1996



$$g(\varepsilon = 0) = 0$$

in all dimensions

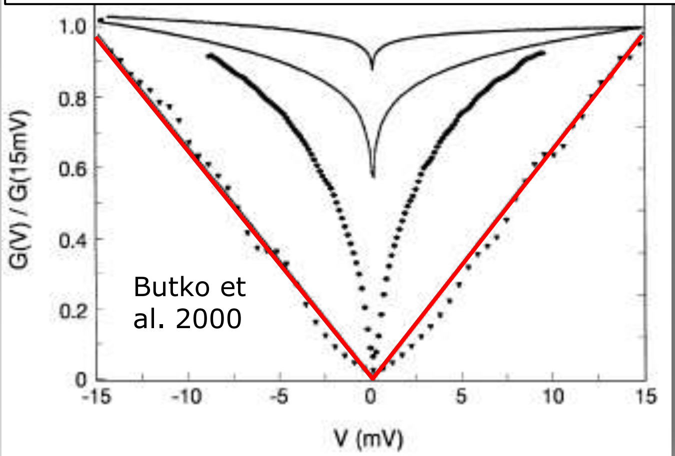
Effect on electron properties

- Low-temperature DC transport

$$\sigma(T) \sim \exp\left(-\sqrt{T_0 / T}\right)$$

- AC transport
- Tunneling
- Heat capacity
- Thermopower
- Relaxation dynamics

Tunneling conductance of Be film



Reviews:
- Efros & Shklovskii, in *Electron-Electron Interactions In Disordered Systems*, 1985
- Pollak & Ortuno, *ibid*.
- Efros, arXiv:cond-mat/0011093

Beyond the “simple” E-S bound

How much does the ES bound overestimates the true DOS?

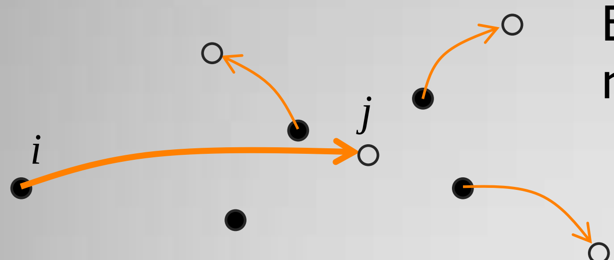
$$g(\varepsilon) \ll \varepsilon^{d-1} \ ?$$

Large parametric difference

Efros, 1976
Baranovskii et al, 1980

By a numerical factor only?

Efros, cond-mat/0011093
Mueller & Pankov, 2007



Energy can be further lowered by local rearrangements – “polaronic effect”

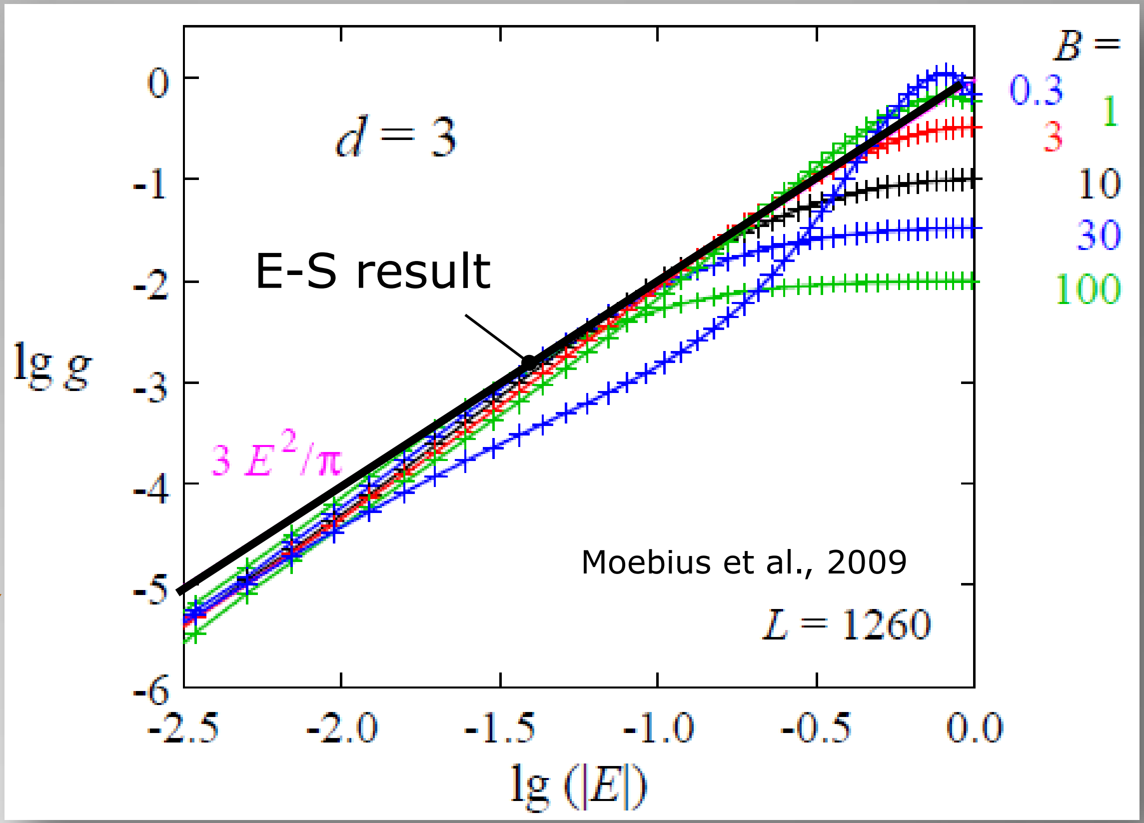
$$E \to E - \Delta E_{\mathrm{pol}}$$

Mott, 1975

Stability condition is $\varepsilon_j - \varepsilon_i - \frac{e^2}{r_{ij}} - \Delta E_{\mathrm{pol}} \geq 0$

Baranovskii et al. 1979; Davies et al. 1983; Levin et al. 1987; Moebius et al. 1992; Vojta et al. 1993; Li & Philips 1994; Pikus & Efros 1994; Overlin et al. 2004; Glatz et al. 2008; Moebius et al. 2009; Surer et al. 2009; Goethe & Palassini 2009; Moebius & Richter, 0908.3092; …

Gigantic system size!



Deviations from the E-S bound are a factor of 2-3 only

Numerical studies in 2D & 3D

Coulomb gap in 1D

Analytical theory

$$\frac{1}{g(\varepsilon)} = \frac{1}{g_0} + Ce^2 \ln \frac{\varepsilon_*}{|\varepsilon|}$$

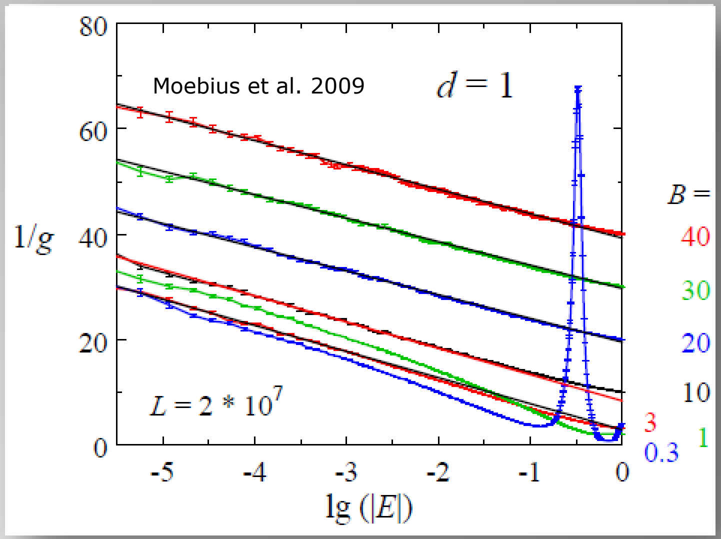
$$C = 1$$

Baranovskii et al, 1980
Raikh & Efros, 1987
Johnson & Khmelnitskii, 1996

$$C = 2$$

Vojta & John, 1993

Simulations



$$C = 1.95 \pm 0.05 \qquad B \geq 10$$

Earlier numerical work:
Moebius et al. 1987
Vojta & John, 1993

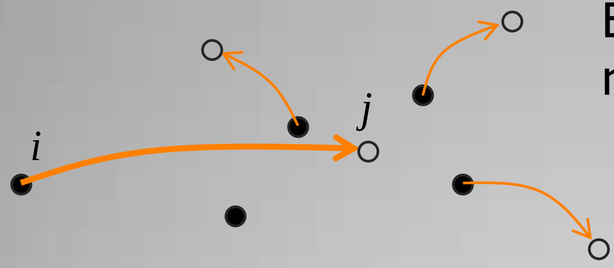
$C = 2.23 \pm 0.05,\ B = 2$

$C = 2.18,\ B = 4$

$C = 2.07,\ B = 16$

- Derive the 1D Coulomb gap rigorously
- Compare with prior mean-field theories
- Reconcile analytical and numerical results

Objectives of this work



Energy can be further lowered by local rearrangements – "polaronic effect"

In 1D, average No. of dipoles excited is

$$N \sim (e^2 g)^2 \ln\left|\frac{\varepsilon_*}{\varepsilon}\right| \sim \frac{1}{\ln|\varepsilon_* / \varepsilon|} \ll 1$$

Compare w/2D and 3D: $N_{2D} \sim 1, \quad N_{3D} \sim \sqrt{\frac{\Delta}{\varepsilon}} \gg 1$

E-S criterion is sufficient in 1D

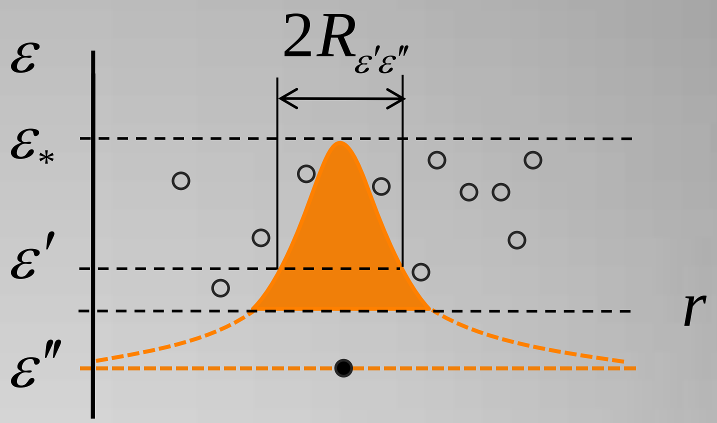
Effective hard-core potential

Stability criterion:

$$r > R_{\varepsilon'\varepsilon''} \equiv e^2 \frac{\theta(-\varepsilon'\varepsilon'')}{|\varepsilon' - \varepsilon''|}$$

can be rewritten as

$$\exp\left(-\beta U_{\varepsilon'\varepsilon''}\right) = 1$$



where we defined the hard-core potential

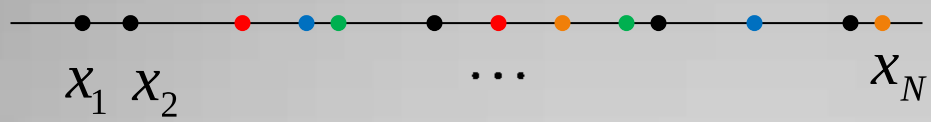
$$U_{\varepsilon'\varepsilon''}(r > R_{\varepsilon'\varepsilon''}) = 0, \quad U_{\varepsilon'\varepsilon''}(r \le R_{\varepsilon'\varepsilon''}) = \infty, \quad \beta = \text{arbitrary}$$

The desired density of states is determined by Boltzmann weight

$$g(E) \propto g_0 \exp\left(-\beta U_{\text{tot}}\right), \quad U_{\text{tot}} = \sum_{i<j} U_{\varepsilon_i \varepsilon_j}$$

Mapping to a multi-component gas

Each localized state $\rightarrow$ a particle on a line of length L
Energy (discretized in some increments $\Delta\varepsilon$) $\rightarrow$ color



Grand partition function

$$Z(L) = \sum_{\{N_\varepsilon\}} \prod_{\varepsilon} \frac{(w_\varepsilon \Delta\varepsilon)^{N_\varepsilon}}{N_\varepsilon!} \prod_{j=1}^{N_\varepsilon} \int_0^L dx_j \, e^{-\beta U_{\text{tot}}}$$

Bare density of states $\rightarrow$ fugacity $w_\varepsilon \Delta\varepsilon, \quad w_\varepsilon = g_0$

Density of states $\quad g(\varepsilon) = \dfrac{n_\varepsilon}{\Delta\varepsilon}$

Grand partition function

$$Z(L) = \sum_{\{N_\varepsilon\}} \prod_{\varepsilon} \frac{(w_\varepsilon \Delta\varepsilon)^{N_\varepsilon}}{N_\varepsilon!} \prod_{j=1}^{N_\varepsilon} \int_0^L dx_j \, e^{-\beta U_{\text{tot}}}$$

Efros 1976, Eq. (20)

$$Z(L) = \sum_{\{N_\varepsilon\}} \prod_{k} \int g_0 d\varepsilon_k \prod_{i,j}^{N_\varepsilon} \Theta(\Delta_i^j)$$

$$\Delta_i^j \equiv \varepsilon_j - \varepsilon_i - \frac{e^2}{r_{ij}}, \quad \text{if } \varepsilon_i < 0 < \varepsilon_j$$

Same as Efros 1976, Eq.(20)

Extracting density of states

Use thermodynamic relation b/w pressure and fugacity

$$g(\varepsilon)\Delta\varepsilon = n_\varepsilon = \left.\frac{\partial\gamma}{\partial \ln w_\varepsilon}\right|_{w_\varepsilon = g_0} \qquad \gamma \equiv \beta p = \frac{p}{T} = \frac{\text{"pressure"}}{\text{"temperature"}}$$

<u>Example</u>: ideal gas

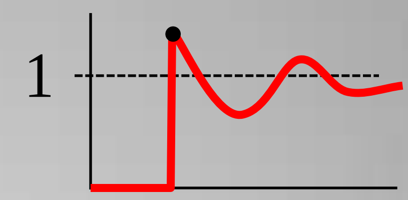
$$\gamma = \frac{p}{T} = \sum_\varepsilon n_\varepsilon\,, \quad \frac{d\ln n_\varepsilon}{d\ln w_\varepsilon} = 1, \quad n_\varepsilon = w_\varepsilon \Delta\varepsilon \quad \therefore \quad g(\varepsilon) = g_0$$

In general, $\boxed{\gamma = \lim_{L\to\infty} \frac{1}{L} \ln Z(L)}$

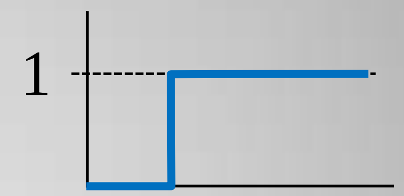
Virial Theorem for a 1D hard-core gas:

$$\gamma = \beta p = \sum_{\varepsilon} n_{\varepsilon} + \sum_{\varepsilon,\varepsilon'} R_{\varepsilon\varepsilon'} G_{\varepsilon\varepsilon'}(R_{\varepsilon\varepsilon'} + 0) n_{\varepsilon} n_{\varepsilon'}$$

$G_{\varepsilon\varepsilon'}(r)$ = two-body correlation function



If correlations are weak, then $G_{\varepsilon\varepsilon'}(r > R_{\varepsilon\varepsilon'}) = 1$



Leads to the transcendental equation

$$n_{\varepsilon} = (w_{\varepsilon} \Delta\varepsilon) e^{-\sum_{\varepsilon'} 2R_{\varepsilon\varepsilon'} n_{\varepsilon'}}$$

$$g(\varepsilon) = g_0 \exp(-A_{\varepsilon}) \qquad A_{\varepsilon} = \int_0^{\varepsilon_*} 2R_{\varepsilon\varepsilon'} g(\varepsilon') d\varepsilon'$$

Similar equation can be derived in higher dimensions

Mean-field theory

Right thing on the first try

$$g(\varepsilon) = g_0 \exp(-A_\varepsilon) \qquad A_\varepsilon = \int_0^{\varepsilon_*} 2R_{\varepsilon\varepsilon'} g(\varepsilon')\, d\varepsilon'$$

This is the **original** self-consistent equation of Efros (1976) and also the BPW mean-field eq. of Vojta & John (1993)

Solution:

$$g(\varepsilon) = \frac{g_0}{1 + Ce^2 g_0 \ln \frac{\varepsilon_*}{|\varepsilon|}}, \quad C = 2$$

Like Raikh & Efros 1987
but with different *C*

Result from numerics:

$$C = 1.95 \pm 0.05$$

Moebius et al. 2009
Vojta & John, 1993
Moebius et al. 1987

SCE v1.0 (1976)

$$g(\varepsilon) = g_0 \exp(-A_\varepsilon)$$

SCE v2.0 (1980-)

$$g(\varepsilon) = g_0 \exp\left(-\frac{1}{2} A_\varepsilon\right)$$

Argument given: to avoid double-counting (?)

Footnote: "In essence, this rule is only empirical. For example, in the region … where g differs little from g_0, we can use perturbation theory and show that the first correction to g_0, which follows from the SCE, is **undervalued by a factor of two**. However, at low energies the result of the SCE agrees well with the computer experiment."

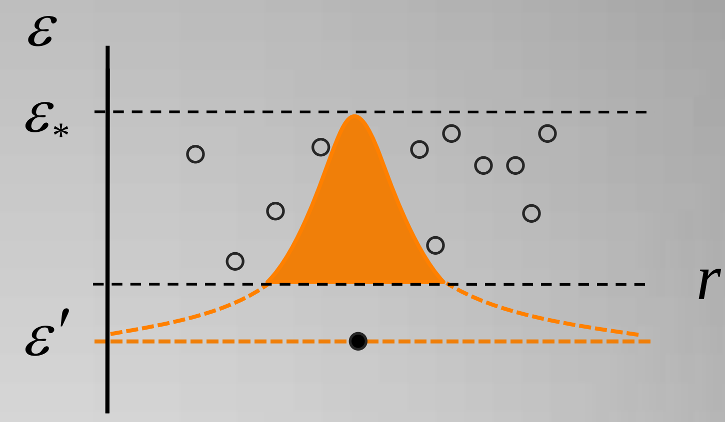
-Baranovskii, Shklovskii & Efros, 1980

2nd try – "empirical correction"

Why does mean-field work?

Excluded area is large:

$$A_\varepsilon = \int_0^{\varepsilon_*} 2R_{\varepsilon\varepsilon'} g_{\varepsilon'}\, d\varepsilon' = \ln \frac{g_\varepsilon}{g_0} \gg 1$$

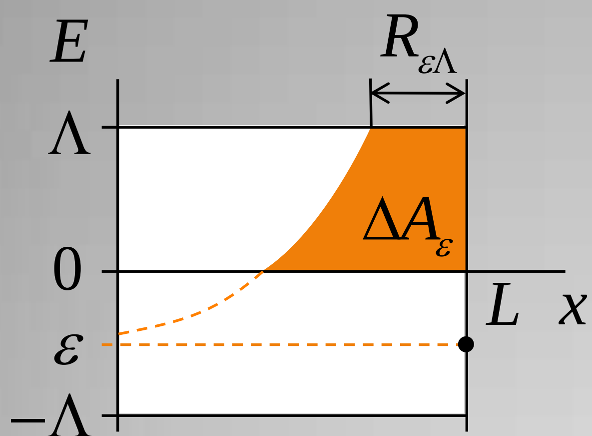


No obvious reason why correlations are weak…

**Hint* : the mean-field theory (that does not include correlations) is saved by the large log,

$$\ln \frac{\varepsilon_*}{|\varepsilon|} \gg 1$$

Step 1: Transfer matrix



$$\frac{\partial}{\partial L} Z(L) = \sum_{|\varepsilon|<\Lambda} \frac{\partial}{\partial L_\varepsilon} Z(A) \Big|_{L_\varepsilon = L}$$

$$A = \text{area defined by } \max x_\varepsilon = L_\varepsilon$$

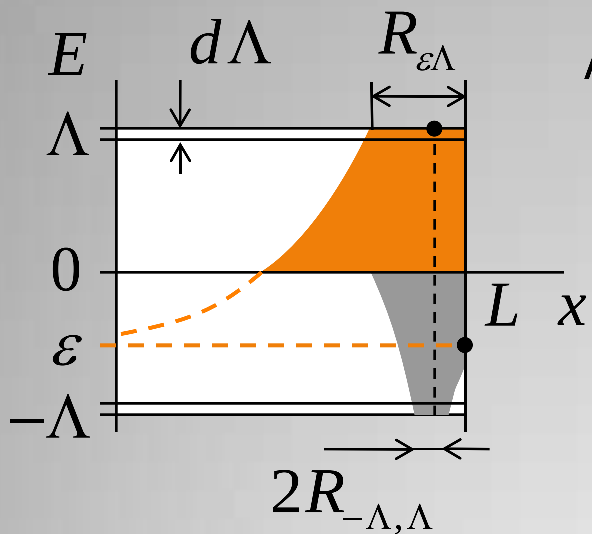
$$\frac{\partial}{\partial L_\varepsilon} Z(A) = (w_\varepsilon \Delta\varepsilon)\, Z(A \setminus \Delta A_\varepsilon)$$

Similar to:
Baxter, 1965

This system of equations is not closed – no exact solution
Approximate closure is provided by the RG technique

Another RG approach was proposed by Johnson & Khmelnitskii, 1996, but our results for *C* disagree

$$Z(A\setminus\Delta A_\varepsilon)=Z(A\setminus\Delta A_{\Lambda-d\Lambda,\varepsilon})-(R_{\Lambda\varepsilon}d\Lambda)\frac{\partial}{\partial L_\Lambda}Z(A\setminus\Delta A_{\Lambda-\Delta\Lambda,\varepsilon})$$



Assuming $e^2 w_\Lambda \ll 1$, we get RG equations

$$\frac{\partial}{\partial\Lambda}\gamma = w_\Lambda + w_{-\Lambda}$$

$$\frac{\partial}{\partial\Lambda}w_\varepsilon = 2R_{\varepsilon,-s\Lambda}w_\varepsilon w_{-s\Lambda}\,,\quad s=\operatorname{sign}\varepsilon$$

After integration, we recover the SCE v1.0!

$$g(\varepsilon)=g_0\exp(-A_\varepsilon)\qquad A_\varepsilon=\int_0^{\varepsilon_*}2R_{\varepsilon\varepsilon'}g(\varepsilon')\,d\varepsilon'$$

Step 2: Renormalization group

Coulomb gap in 1D

Analytical theory

$$\frac{1}{g(\varepsilon)} = \frac{1}{g_0} + Ce^2 \ln \frac{\varepsilon_*}{|\varepsilon|}$$

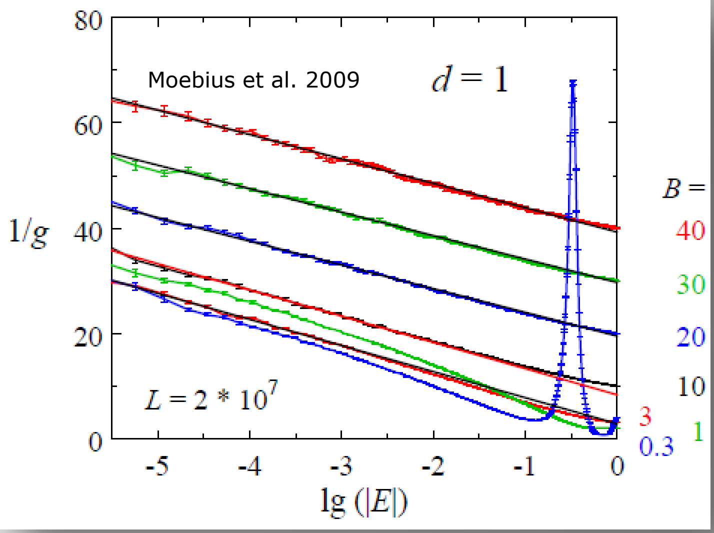
$$C = 1$$

Baranovskii et al, 1980
Raikh & Efros, 1987
Johnson & Khmelnitskii, 1996

$$C = 2$$

Present work
Also: Vojta & John, 1993

Simulations



$$C = 1.95 \pm 0.05$$

Earlier numerical work:
Moebius et al. 1987
Vojta & John, 1993

Conclusions & outlook

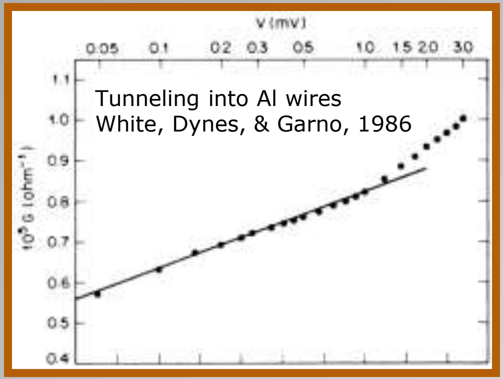
- Classical 1D Coulomb gap problem has been solved in a controlled way
- The result agrees with Efros 1976, not its later revision
- Discrepancy with numerical work has been reconciled

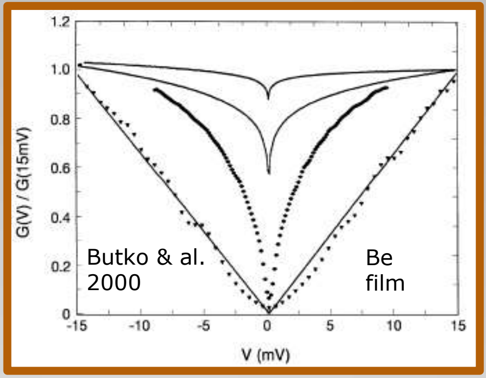
<u>Possible future directions</u>

- Thermal & quantum effects:
  - Finite T smears the Coulomb gap — Mogilyanskii & Raikh 1989
  - Classical Coulomb gap + Luttinger-liquid = ?
- Higher dimensions, $d = 1 + \epsilon$, via ϵ-expansion
- Comparison with experiments

Experimental probes of C-Gap

- Tunneling: most successful so far





Difficult to avoid screening by the source electrode

- Photoemission: time to renew the efforts?