

# WEAK COUPLINGS IN THE ONE-COMPONENT PLASMA IN TWO DIMENSIONS FOR A DISK WITH A CENTERED IMPENETRABLE NEUTRALIZING CHARGE

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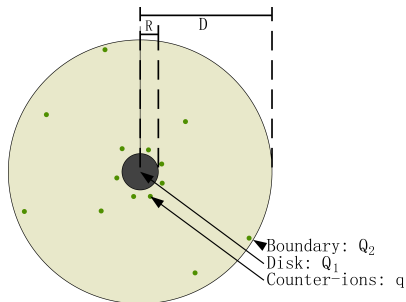
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*Departamento de Física*

**Universidad de los Andes**

# Problem statement



**Figure :** The 2D cell model. The disk with charge  $Q_1$  and radius  $R$  is surrounded by counter-ions of charge  $-q$  enclosed by an exterior boundary at  $D$  with charge  $Q_2$ .

ion-disk: Manning parameter

$$\xi = \frac{1}{2} \beta Q_1 q \propto \frac{N}{T}. \quad (1)$$

ion-ion: coupling parameter  $\Gamma$

$$\Xi = \frac{1}{2} \beta q^2 \propto \frac{1}{T}. \quad (2)$$

Often recalled  $\Gamma$  in the literature

ion-boundary:

$$\xi_B = \frac{1}{2} \beta Q_2 q \propto \frac{N}{T}. \quad (3)$$

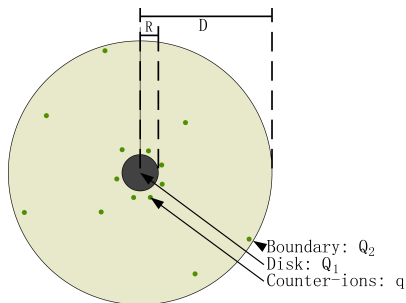
Same meaning as the Manning parameter

lateral extension parameter

$$\Delta = \log \frac{D}{R}. \quad (4)$$

# Problem statement

$$\beta H = 2\xi \sum_{j=1}^N \log \left| \frac{\mathbf{r}_j}{R} \right| - 2\Xi \sum_{1 \leq j < k \leq N} \log \left| \frac{\mathbf{r}_j - \mathbf{r}_k}{R} \right| + \underbrace{\frac{[N\Xi - \xi]^2}{\Xi} \Delta + N\Xi \log \frac{R}{L}}_{\tilde{E}_B} \quad (1)$$



**Figure :** The 2D cell model. The disk with charge  $Q_1$  and radius  $R$  is surrounded by counter-ions of charge  $-q$  enclosed by an exterior boundary at  $D$  with charge  $Q_2$ .

## Neutrality and the thermodynamic limit

Neutrality  $N\Xi = \xi + \xi_B$ .

The thermodynamic limit, or  $N \rightarrow \infty$ , is equivalent to  $\Xi \rightarrow 0$  at constant  $\xi$  and  $\xi_B$

# Different cases

- $\Xi \rightarrow 0$
- $\Xi \rightarrow \infty$
- ‡  $\Xi$  is a whole number

## Characteristics

Mean field theory, to this problem often attributed to Fuoss et al. (1951), Katchalsky et al. (1953). To our problem it is equivalent to  $\Xi \rightarrow 0$

**Method:** Poisson-Boltzmann equation

# Different cases

- $\Xi \rightarrow 0$
- $\Xi \rightarrow \infty$
- ‡  $\Xi$  is a whole number

## Characteristics

The strong coupling regime (Šamaj and Trizac 2011a;b)

**Method:** Wigner Strong Coupling approach

# Different cases

- $\Xi \rightarrow 0$
- $\Xi \rightarrow \infty$
- ‡  $\Xi$  is a whole number

## Characteristics

**Method:** Analytic

- ▶  $\Xi = 1$ : Free fermion (Deutsch and Lavaud 1974, Deutsch et al. 1979, Jancovici 1981)
- ▶  $\Xi = 2, 3, \dots$  method proposed by Šamaj et al. (1994)

# Different cases

- $\Xi \rightarrow 0$
- $\Xi \rightarrow \infty$
- ‡  $\Xi$  is a whole number
- ★  $\Xi$  is small

## Objectives

The weak coupling regime (Burak and Orland 2006)

- ▶ Determine  $\mathcal{Z}$
- ▶ Derive the profile
- ▶ Recover mean field results
- ▶ Determine condensation (MF  $\rightarrow$   
 $f_M = 1 - 1/\xi$ )

# The partition function $\mathcal{Z}$

$$\mathcal{Z}_N = \int \mathbf{d}^{2N} r e^{-\beta H(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)}. \quad (2)$$

Using a complex variable notation the Hamiltonian reads,

$$\beta H = 2\xi \sum_{j=1}^N \log \|z_j\| - \Xi \sum_{1 \leq j < k \leq N} \log [(z_j - z_k)(\bar{z}_j - \bar{z}_k)] + \tilde{E}_B, \quad (3)$$

and the partition function is rewritten as,

$$\mathcal{Z}_N \propto \int \mathbf{D}^N z \left[ \prod_{1 \leq j < k \leq N} \|z_j - z_k\|^2 \right]^\Xi \prod_{j=1}^N \|z_j\|^{-2\xi}. \quad (4)$$



# The partition function $\mathcal{Z}$

$$\mathcal{Z}_N \propto \int \mathbf{D}^N z \left[ \prod_{1 \leq j < k \leq N} \|z_j - z_k\|^2 \right]^{\Xi} \prod_{j=1}^N \|z_j\|^{-2\xi}. \quad (2)$$

Which brings us back to  $\Xi \in \{1, 2, \dots\}$  since,

$$\left[ \prod_{1 \leq j < k \leq N} (z_j - z_k) \right] = \text{Det} [V_{N \times N}], \quad (3)$$

with

$$V_{N \times N} = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ z_1 & z_2 & z_3 & \dots & z_N \\ z_1^2 & z_2^2 & z_3^2 & \dots & z_N^2 \\ \cdot & \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot \\ z_1^{N-1} & z_2^{N-1} & z_3^{N-1} & \dots & z_N^{N-1} \end{bmatrix} \quad (4)$$

# Weak coupling approximation

Proposed by Burak and Orland (2006),

$$2 \log |\mathbf{r}_1 - \mathbf{r}_2| = \log \|\mathbf{r}_1\| + \log \|\mathbf{r}_2\| + \log [2 \cosh (\log \|\mathbf{r}_1\| - \log \|\mathbf{r}_2\|) - 2 \cos \theta_{12}] \approx 2 \log |\mathbf{r}_>|, \quad (5)$$

transforming the Hamiltonian to,

$$\beta H \approx \frac{2\xi}{\Xi} \sum_{j=1}^N y_j - 2 \sum_{1 \leq j < k \leq N} y_{>}^{(j,k)} + \tilde{E}_B, \quad (6)$$

with  $y = \Xi \log(r/R)$  (a.k.a. *centrifugal variables*).

- ★ Distance between particles is large
- ★ Dropped angular correlations
- ★  $\Xi$  needs to be small
- ★ 2D  $\rightarrow$  1D.
- ★  $y_{>}$  suggests arrangement

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Departing from the base order, denoted by **[BO]**,  $y_1 < y_2 < \dots < y_N$ , the  $N$ -dimensional phase space is mapped entirely from permutations of such arrangement.

# Weak coupling $\mathcal{Z}$

Written in terms of the  $\{y_k\}$  variables,

$$\mathcal{Z}(\Xi, \xi, N, \Delta) = \left( \frac{2\pi R^2}{\Xi} \right)^N \int \mathbf{d}^N y e^{-\beta H + \frac{2}{\Xi} \sum_{j=1}^N y_j}, \quad (7)$$

transforms to,

$$\mathcal{Z}(\Xi, \xi, N, \Delta) = e^{-\tilde{E}_B} \left( \frac{2\pi R^2}{\Xi} \right)^N N! \int_0^{\Xi\Delta} \mathbf{d}y_N \int_0^{y_N} \mathbf{d}y_{N-1} \dots \int_0^{y_2} \mathbf{d}y_1 e^{-\mathcal{H}}, \quad (8)$$

with

$$\mathcal{H} = \frac{2(\xi - 1)}{\Xi} \sum_{j=1}^N y_j - 2 \sum_{1 \leq j < k \leq N} y_k = \sum_{j=1}^N \left[ \frac{2(\xi - 1)}{\Xi} - 2(j - 1) \right] y_j \quad (9)$$

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with

$$\mathcal{H} = \sum_{j=0}^N a_j (y_{j+1} - y_j) - a_N \Xi \Delta, \quad (9)$$

choosing  $y_0 = 0$  and  $y_{N+1} = \Xi\Delta$ , and,

$$a_j = \left[ j - \left( \frac{\xi - 1}{\Xi} + \frac{1}{2} \right) \right]^2 = \left[ j - \left( \frac{f_M}{1 + \frac{\xi_B}{\xi}} N + \frac{1}{2} \right) \right]^2 = [j - \sqrt{a_0}]^2 \quad (10)$$

**Rationale:** Use the Laplace transformation to find the partition function Burak and Orland (2006).

# Weak coupling $\mathcal{Z}$

Using the notation  $f_j(x) = e^{-a_j x}$ ,

$$\mathcal{Z}(\Xi, \xi, N, \Delta) = \left( \frac{2\pi R^2}{\Xi} \right)^N N! e^{a_N \Xi \Delta - \tilde{E}_B} \times \underbrace{\int_0^{\Xi \Delta} dy_N \int_0^{y_N} dy_{N-1} \dots \int_0^{y_2} dy_1 \prod_{j=0}^N f_j(y_{j+1} - y_j)}_{[f_N \otimes f_{N-1} \otimes \dots \otimes f_1 \otimes f_0](\Xi \Delta)}.$$
(11)

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$$\mathcal{T}_{\{f_N \otimes \dots \otimes f_0\}}^{[\Xi \Delta]}(s) = \prod_{j=0}^N \frac{1}{s + a_j} \quad (12)$$

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Leading to the inverse

- ▶ Anticipating,  $\mathcal{Z} \propto \sum_j e^{-a_j \Xi \Delta}$
- ▶  $\Delta$  needs to be large
- ▶  $\mathcal{Z} \sim e^{-a_{j^*} \Xi \Delta}$
- ▶  $\{a_j\}$ 's may be degenerate



# Who is $j^*$

$j^*$  is the integer closes to  $\sqrt{a_0}$ .

$$\sqrt{a_0} = \frac{\xi - 1}{\Xi} + \frac{1}{2} = \frac{f_M}{1 + \frac{\xi_B}{\xi}} N + \frac{1}{2}$$

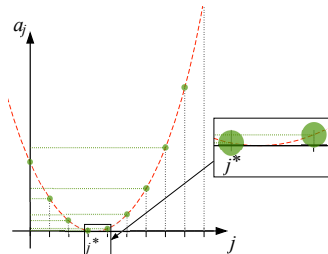


Figure : Artistic representation of  $a_j$  as a function of  $j$  with  $j^*$  the location of the minimum

# Who is $j^*$

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$$j^* = \left\lceil \frac{\xi - 1}{\Xi} \right\rceil = \left\lceil \frac{f_M N}{1 + \frac{\xi_B}{\xi}} \right\rceil. \quad (13)$$

## Condensation

Notice how

$$\frac{j^*}{N} \rightarrow \frac{f_M}{1 + \frac{\xi_B}{\xi}}$$

in the thermodynamic limit

## Transitions

Since  $\mathcal{Z} \sim e^{-a_{j^*} \Xi \Delta}$  then at a change in  $j^*$  the behavior of the system will change!

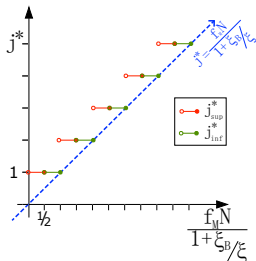


Figure : The value for  $j^*$  as a function of  $f_M N / (1 + \xi_B / \xi)$ .

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## Degeneracy

Depends if

$$\frac{2}{\Xi} (1 + \xi_B) \in \mathbb{N},$$

which will be even or odd

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$$\mathcal{T}_{\{f_N \otimes \dots \otimes f_0\}}^{[\Xi \Delta]}(s) = \prod_{j=0}^N \frac{1}{s + a_j}$$

$$\mathcal{Z}(\Xi, \xi, N, \Delta) = \left( \frac{2\pi R^2}{\Xi} \right)^N N! e^{a_N \Xi \Delta - \tilde{E}_B} \sum_{j=0}^N \underbrace{\left[ \prod_{k=0, k \neq j}^N \frac{1}{a_k - a_j} \right]}_{\text{Defined as } C_{0, N; j}} e^{-a_j \Xi \Delta}. \quad (14)$$

## Non-degenerate case

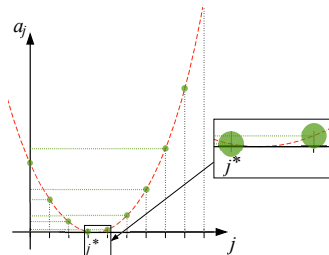


Figure : Artistic representation of  $a_j$  as a function of  $j$  with  $j^*$  the location of the minimum

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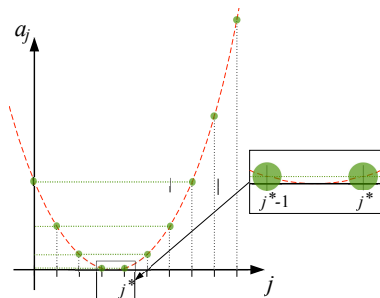
Degeneracy

Depends if

$$\frac{2}{\Xi} (1 + \xi_B) \in \mathbb{N},$$

which will be even or odd

## Even degenerate case



**Figure :** Artistic representation of  $a_j$  as a function of  $j$  with  $j^*$  the location of the minimum with  $2(1 + \xi_B)/\Xi$  an even number.

# Who is $j^*$

$j^*$  is the integer closes to  $\sqrt{a_0}$ .

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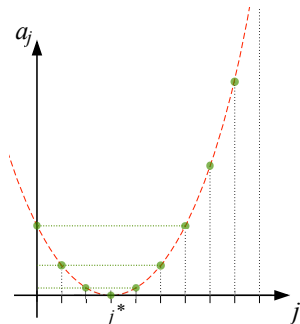
Degeneracy

Depends if

$$\frac{2}{\Xi} (1 + \xi_B) \in \mathbb{N},$$

which will be even or odd

## Odd degenerate cases



**Figure :** Artistic representation of  $a_j$  as a function of  $j$  with  $j^*$  the location of the minimum with  $\frac{2(1 + \xi_B)}{\Xi}$  an odd number

# Who is $j^*$

$j^*$  is the integer closes to  $\sqrt{a_0}$ .

$$j^* = \left\lceil \frac{\xi - 1}{\Xi} \right\rceil = \left\lceil \frac{f_M N}{1 + \frac{\xi_B}{\xi}} \right\rceil. \quad (13)$$

## Degeneracy

Depends if

$$\frac{2}{\Xi} (1 + \xi_B) \in \mathbb{N},$$

which will be even or odd

**Degenerate cases** Due to the **continuity** of the free energy  $\rightarrow$  the partition function, they are a limiting behavior of the non-degenerate scenario.

# The free energy

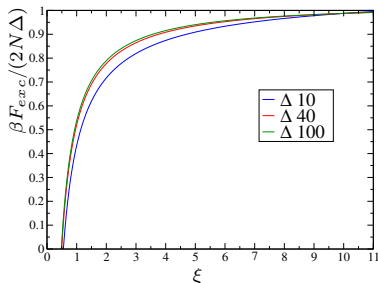
The excess free energy is,

$$\beta F_{exc}(N, \Delta, \xi, \Xi) = -\log \left[ \frac{1}{V} \mathcal{Z}(\Xi, \xi, N, \Delta) \right], \quad (14)$$

keeping in mind,

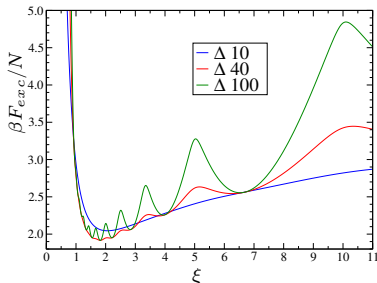
$$\mathcal{Z}(\Xi, \xi, N, \Delta) = \underbrace{\left( \frac{2\pi R^2}{\Xi} \right)^N N! e^{a N \Xi \Delta - \tilde{E}_B}}_1 \underbrace{\sum_{j=0}^N C_{0,N;j} e^{-a_j \Xi \Delta}}_2. \quad (15)$$

**Dominant behavior**



**Figure :** The excess free energy dominant term coming from 1 for  $N = 10$  and  $\xi_B = 0$

**Subdominant behavior**



**Figure :** The excess free energy sub-dominant term coming from 2 for  $N = 10$  and  $\xi_B = 0$



# Density profile

As for the profile,

$$\rho = \frac{N}{\mathcal{Z}(\Xi, \xi, N, \Delta)} \int d^N \mathbf{r} \delta(\mathbf{r} - \mathbf{r}_1) e^{-\beta H} = \frac{\Xi}{2\pi R^2 e^{2y/\Xi}} \rho_y, \quad (16)$$

with

$$\rho_y := N \langle \delta(y - y_1) \rangle_{\{y_j\}}. \quad (17)$$

Since the average must be consistent with the **[BO]**. Hence,

$$\rho_y = \langle \delta(y - y_1) \rangle_{\{y_j\}}^T + \langle \delta(y - y_2) \rangle_{\{y_j\}}^T + \cdots + \langle \delta(y - y_N) \rangle_{\{y_j\}}^T, \quad (18)$$

and,

$$\langle \delta(y - y_k) \rangle_{\{y_j\}}^T = \left( \frac{2\pi R^2}{\Xi} \right)^N \frac{e^{-\tilde{E}_B} N!}{\mathcal{Z}(\Xi, \xi, N, \Delta)} \int_{\mathbf{[BO]}} d^N y \delta(y - y_k) e^{-\mathcal{H}'} \quad (19)$$

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and,

$$\langle \delta(y - y_k) \rangle_{\{y_j\}}^T = \frac{\left\{ \sum_{j=k}^N C_{k,N;j} e^{-a_j(\Xi\Delta - y)} \right\} \left\{ \sum_{j=0}^{k-1} C_{0,k-1;j} e^{-a_j y} \right\}}{\sum_{j=0}^N C_j e^{-a_j \Xi \Delta}} \quad (18)$$

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## Characteristics

- ★ Upfront decay of  $1/r^2$  (MF)
- ★ Behavior near  $R$
- ★ Behavior near  $D$
- ▶ Condensation  $\Rightarrow j^*$

# Density profile

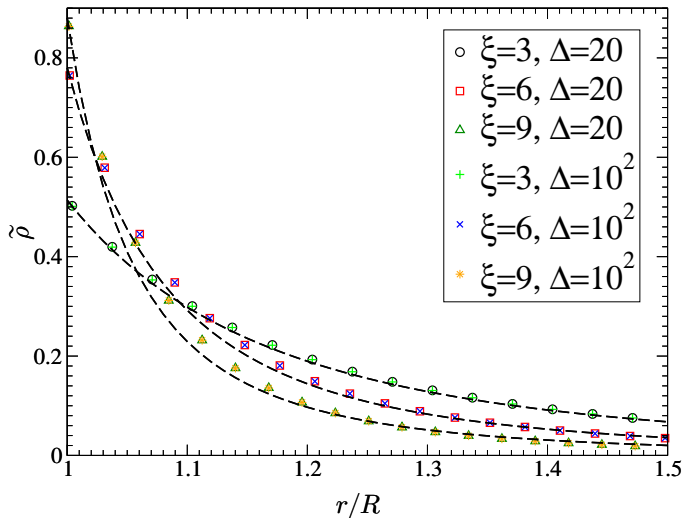


Figure : The density profile  $\tilde{\rho} = 2\pi R^2 \rho / (N\xi)$  near the charged disk for different values of the Manning parameter for  $N = 10$  and  $\xi_B = 0$ .

# Density profile at infinite dilution

Near  $R$ , ( $k \leq j^*$ )

$$\langle \delta(y - y_k) \rangle_{\{y_j\}}^T \simeq \sum_{j=0}^{k-1} \frac{C_{0,k-1;j}}{C_{0,k-1;j^*}} e^{-(a_j - a_{j^*})y} + \mathcal{O}(e^{-\Xi\Delta}), \quad (19)$$

and for the exterior shell ( $k > j^*$ ),

$$\langle \delta(y - y_k) \rangle_{\{y_j\}}^T \simeq \sum_{j=k}^N \frac{C_{k,N;j}}{C_{k,N;j^*}} e^{-(a_j - a_{j^*})(\Xi\Delta - y)} + \mathcal{O}(e^{-\Xi\Delta}). \quad (20)$$

# Density profiles near mean field

At infinite dilution, using  $\tilde{\rho} = 2\pi R^2 \rho / (N\xi)$ ,

$$\tilde{\rho} = \frac{\Xi e^{-2y/\Xi}}{N\xi} \sum_{k=1}^{j^*} \left\{ \sum_{j=0}^{k-1} \frac{C_{0,k-1;j}}{C_{0,k-1;j^*}} \right\} e^{-(a_j - a_{j^*})y} \rightarrow \frac{f_M^2}{1 + \frac{\xi_B}{\xi}} \left( \frac{\tilde{R}}{r} \right)^2 \frac{1}{\left( 1 + (\xi - 1) \log \frac{\tilde{r}}{\tilde{R}} \right)} \quad (21)$$

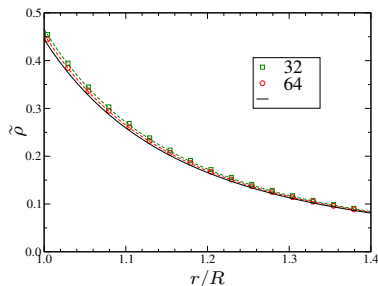


Figure : Density profile  $\tilde{\rho} = 2\pi R^2 \rho / (N\xi)$  for  $\xi = 3$  and  $\Delta = 100$ .

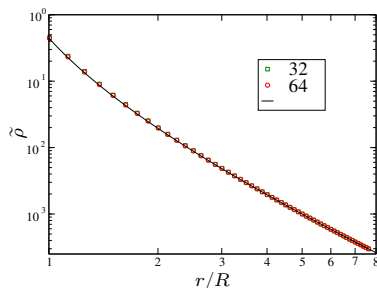


Figure : Same as the figure to the left with logarithmic scales on both axis.

# Contact densities

As for the value of the densities at contact, at  $R$  it gives

$$\tilde{\rho}|_{y=0} = \left( f_M - \left[ f_M - \frac{j^*}{N} \right] \right) \left( f_M + \left[ f_M - \frac{j^*}{N} \right] + \frac{1}{N} \right), \quad (22)$$

and for  $D$ ,

$$e^{2\Delta} \tilde{\rho}|_{y=\Delta} = \frac{1}{N\xi} (a_N - a_{j^*}) = \left( \frac{1}{\xi} - \left[ f_M - \frac{j^*}{N} \right] - \frac{1}{N} \right) \left( \frac{1}{\xi} + \left[ f_M - \frac{j^*}{N} \right] \right), \quad (23)$$

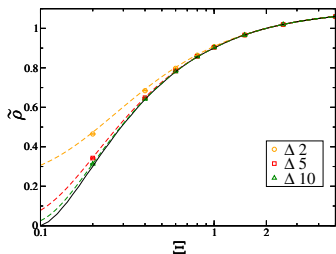


Figure : The density  $\tilde{\rho}$  at contact in  $r = R$  for  $N = 10$  and  $\xi_B = 0$ .

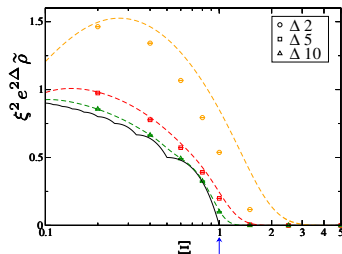
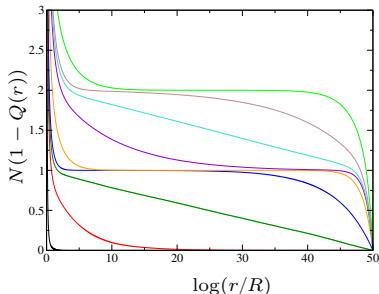


Figure : The density  $\tilde{\rho}$  at contact in  $r = D$  for  $N = 10$  and  $\xi_B = 0$ .

# Integrated charge

- ▶ Mean field behavior at large distances?
- ▶ Condensation
- ▶ Linear form at the transitions
- ▶ Full condensation for  $\Xi > 1 \Rightarrow$   
Strong couplings



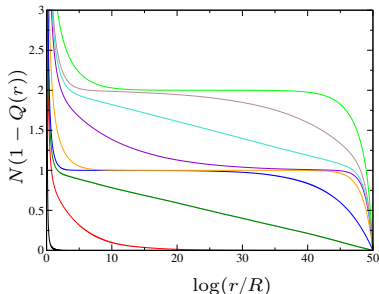
**Figure :** The integrated charge  $N(1 - Q(r))$  as a function of the logarithmic distance for  $\Delta = 10^2$ ,  $\xi_B = 0$  and  $N = 10$  for various  $\Xi$ . The plots read for the coupling parameter from top to bottom  $\Xi = \frac{2}{5}, \frac{10}{21}, \frac{1}{2}, \frac{10}{19}, \frac{2}{3}, \frac{10}{11}, 1, \frac{10}{9}$  and 2.



# Integrated charge

- ▶ Mean field behavior at large distances?
- ▶ **Condensation**
- ▶ Linear form at the transitions
- ▶ Full condensation for  $\Xi > 1 \Rightarrow$   
**Strong couplings**

$$f_{2D} = \frac{j^*}{N} \quad (24)$$

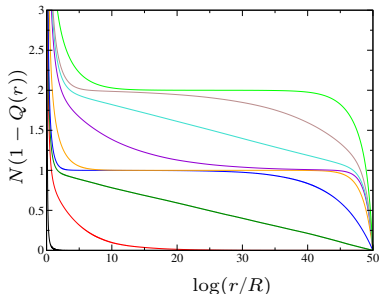


**Figure :** The integrated charge  $N(1 - Q(r))$  as a function of the logarithmic distance for  $\Delta = 10^2$ ,  $\xi_B = 0$  and  $N = 10$  for various  $\Xi$ . The plots read for the coupling parameter from top to bottom  $\Xi = \frac{2}{5}, \frac{10}{21}, \frac{1}{2}, \frac{10}{19}, \frac{2}{3}, \frac{10}{11}, 1, \frac{10}{9}$  and 2.

# Integrated charge

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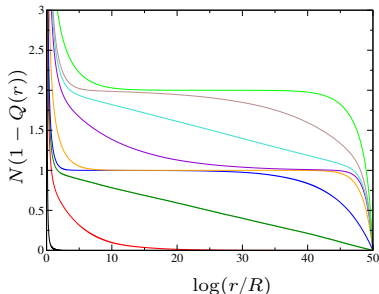
At the transition the  $j^{\text{th}}$  particle is **not** condensed



**Figure :** The integrated charge  $N(1 - Q(r))$  as a function of the logarithmic distance for  $\Delta = 10^2$ ,  $\xi_B = 0$  and  $N = 10$  for various  $\Xi$ . The plots read for the coupling parameter from top to bottom  $\Xi = \frac{2}{5}, \frac{10}{21}, \frac{1}{2}, \frac{10}{19}, \frac{2}{3}, \frac{10}{11}, 1, \frac{10}{9}$  and 2.

# Integrated charge

- ▶ Mean field behavior at large distances?
- ▶ Condensation
- ▶ Linear form at the transitions
- ▶ Full condensation for  $\Xi > 1 \Rightarrow$   
Strong couplings
- ▶ Mean field result is recovered in the thermodynamic limit

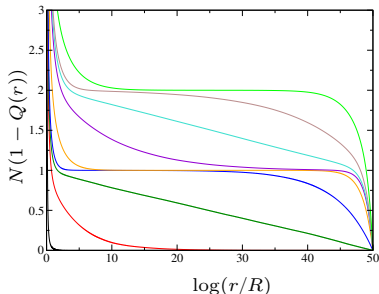


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# Integrated charge

- ▶ Mean field behavior at large distances?
- ▶ Condensation
- ▶ Linear form at the transitions
- ▶ Full condensation for  $\Xi > 1 \Rightarrow$   
Strong couplings

$$f_{2D} \rightarrow f_M \quad (24)$$



**Figure :** The integrated charge  $N(1 - Q(r))$  as a function of the logarithmic distance for  $\Delta = 10^2$ ,  $\xi_B = 0$  and  $N = 10$  for various  $\Xi$ . The plots read for the coupling parameter from top to bottom  $\Xi = \frac{2}{5}, \frac{10}{21}, \frac{1}{2}, \frac{10}{19}, \frac{2}{3}, \frac{10}{11}, 1, \frac{10}{9}$  and 2.

# Conclusions

- ▶ Showed an equivalent 1D problem of the 2D system
- ▶ With some effort we computed  $\mathcal{Z}$  and  $\rho$
- ▶ Recovered mean field results from our assumptions
- ▶ Determined condensation

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Thank you for your attention!