Large deviations for non-interacting trapped fermions

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in collaboration with

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PRL 114, 110402 (2015); EPL 112, 60001 (2015); PRA 94, 063622 (2016)

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J. Stat. Mech., 063301 (2017)
arXiv:1706.03598

this talk

Ultra-cold atoms in confining potentials

- Recent progress in the experimental manipulation of cold atoms

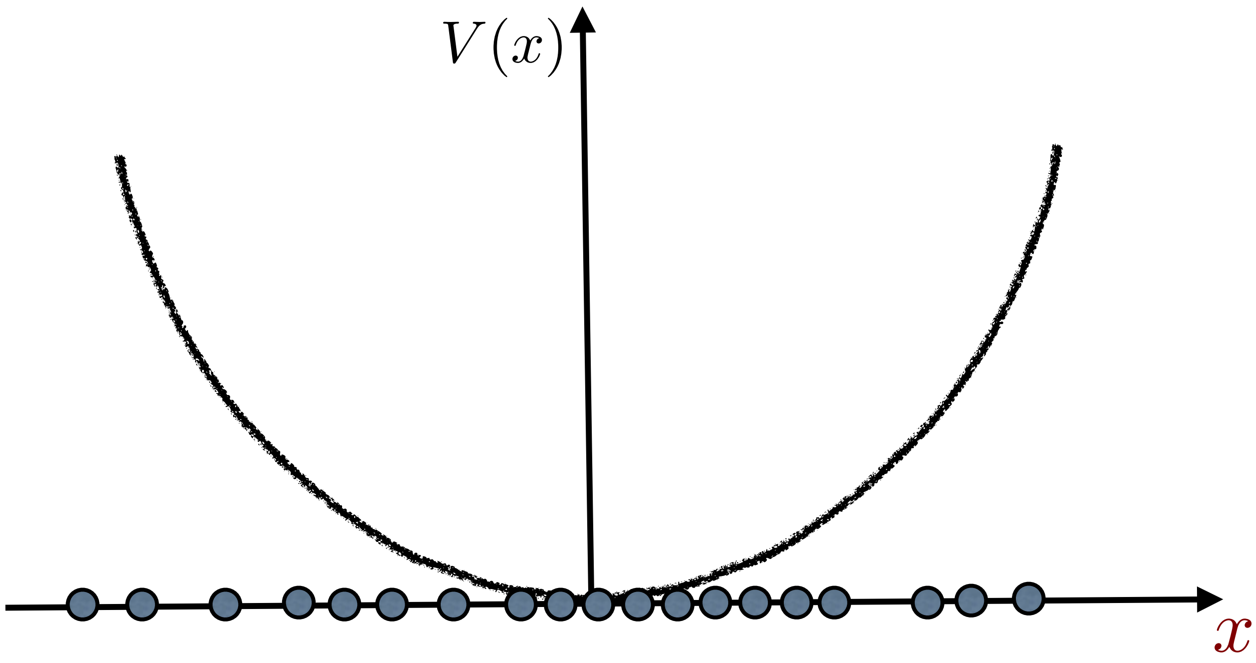
⇒ to investigate the interplay between quantum and thermal behaviors in many-body systems at low temperature

Ultra-cold atoms in confining potentials

- Recent progress in the experimental manipulation of cold atoms

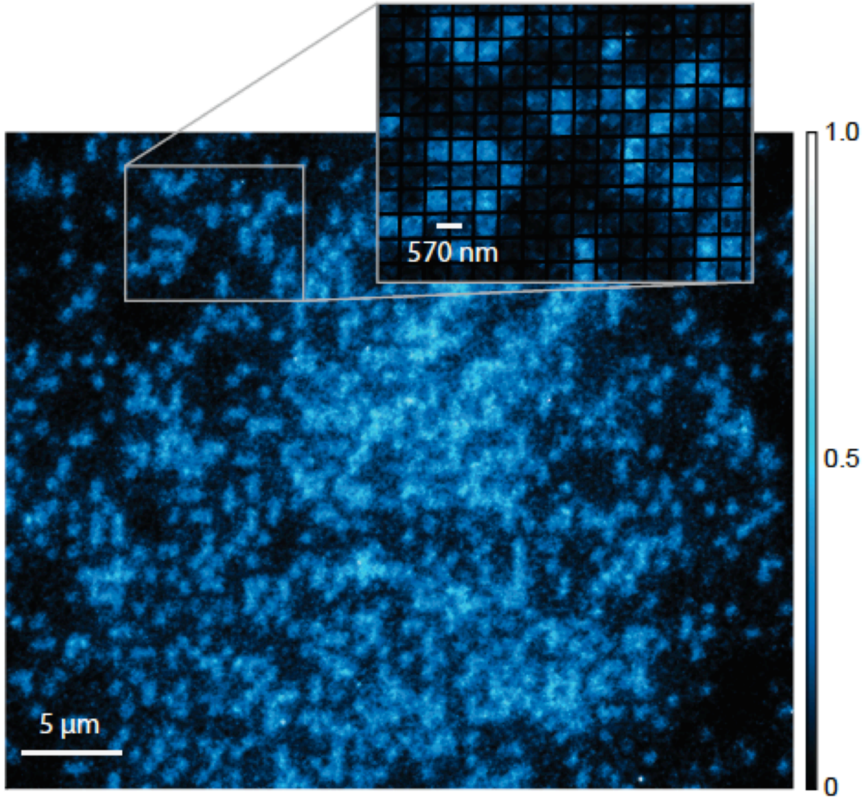
  ⇨ to investigate the interplay between quantum and thermal behaviors in many-body systems at low temperature

- A common feature of these experiments: presence of a confining potential that traps the atoms within a limited spatial region



Quantum Fermi gas microscope

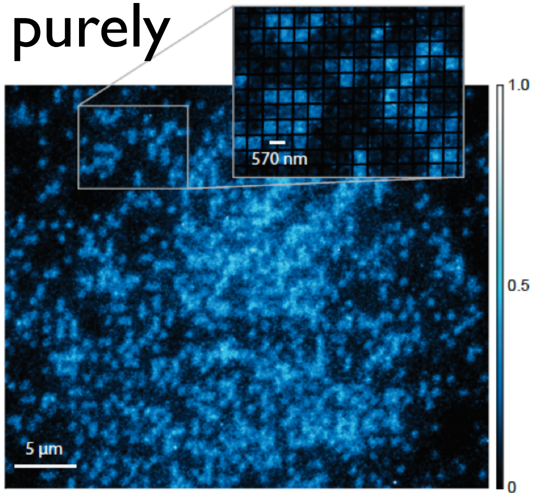
- Direct imaging of spatial fluctuations of the positions of fermions



M. Greiner et al., PRL 2015

Tuning the interactions

- Reaching the non-interacting limit to probe purely quantum effects



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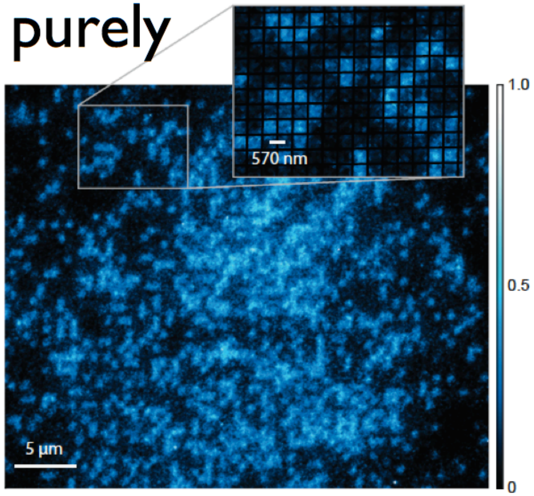
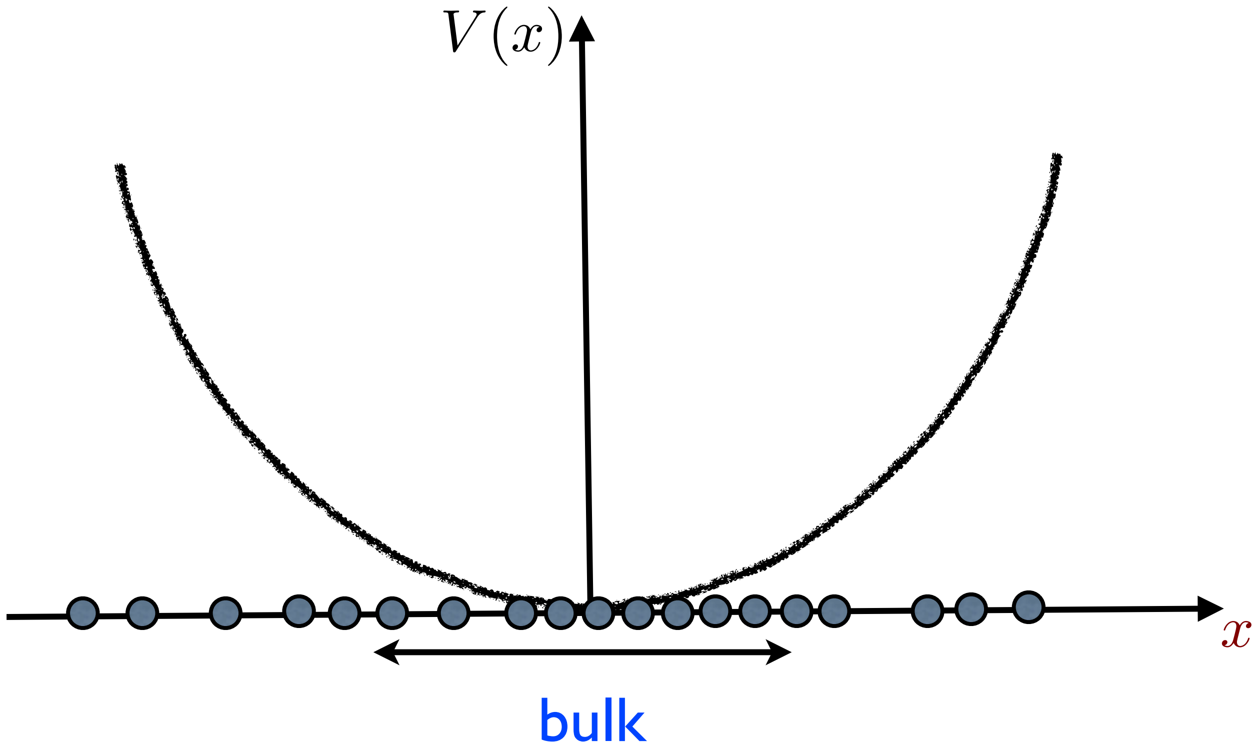


- Interesting quantum many-body effects even in the absence of interactions

Bosons: Bose-Einstein condensation

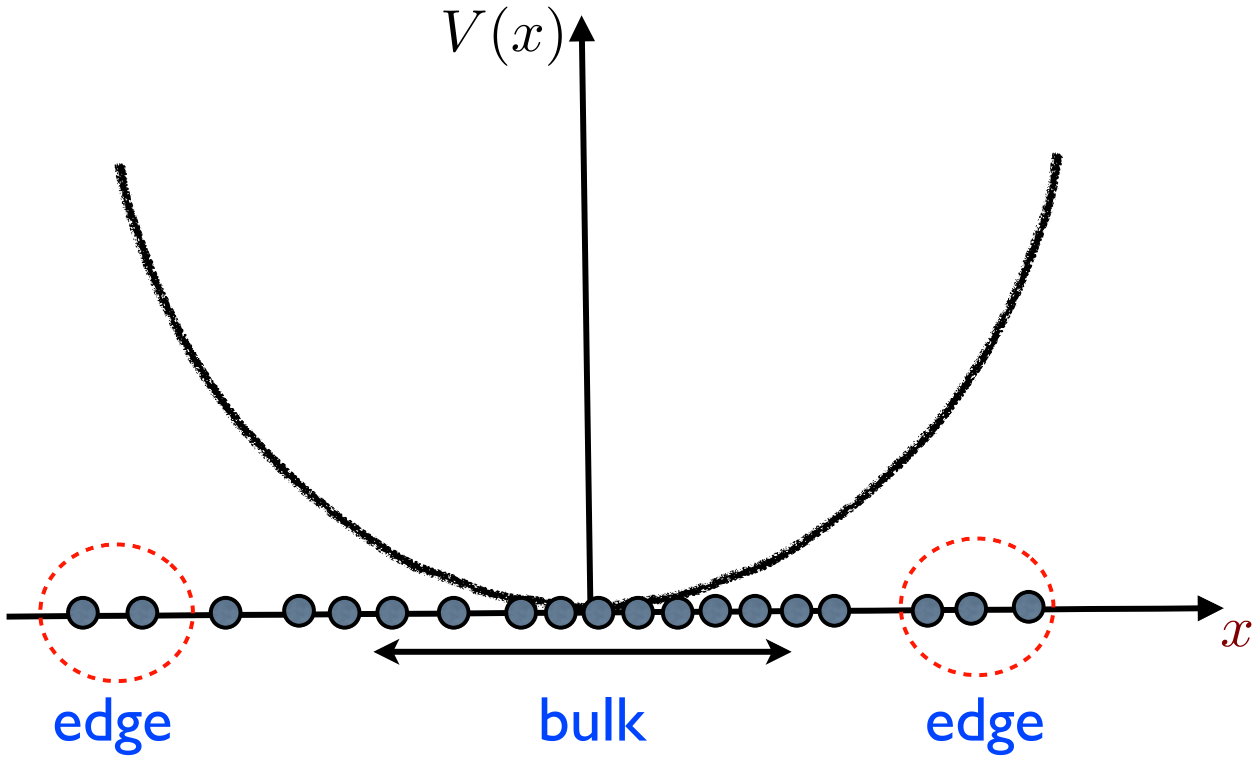
Fermions: Pauli exclusion principle ⟹ rich quantum many-body physics

Ultra-cold atoms in confining potentials



- bulk: traditional many-body physics (translationally invariant system)

Ultra-cold atoms in confining potentials



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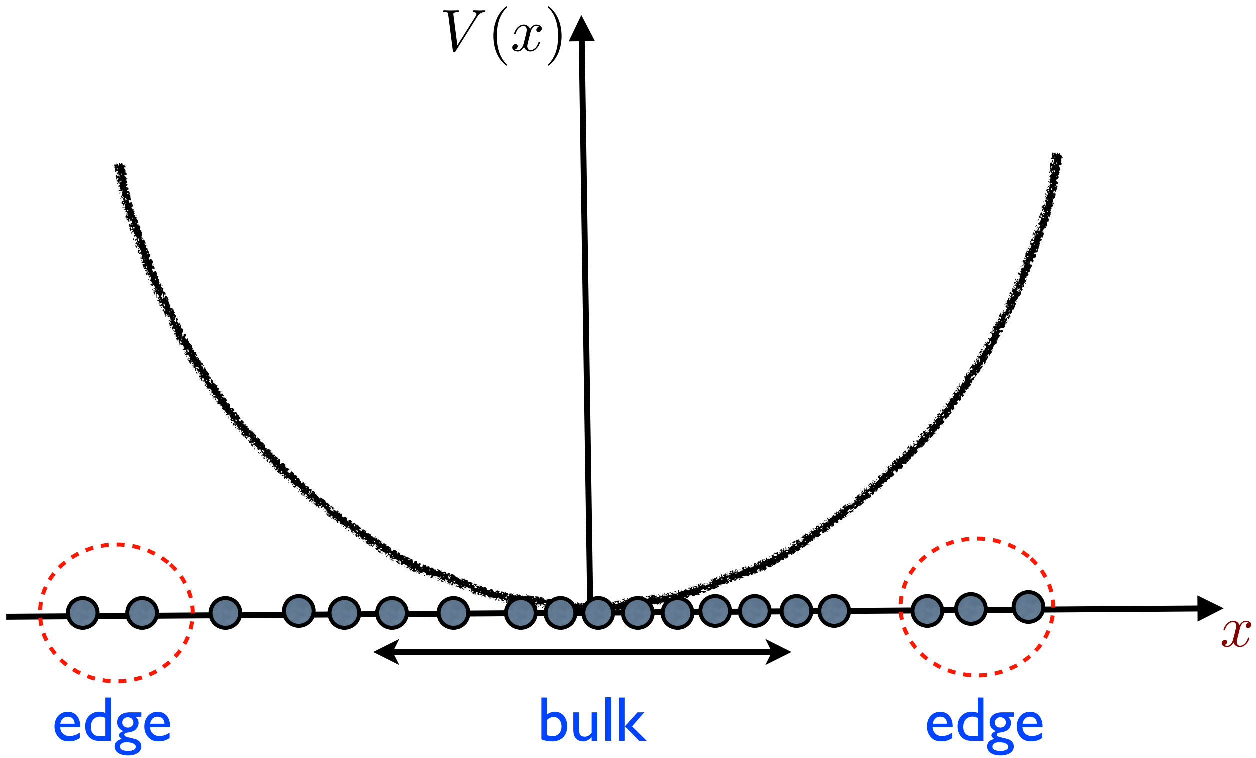
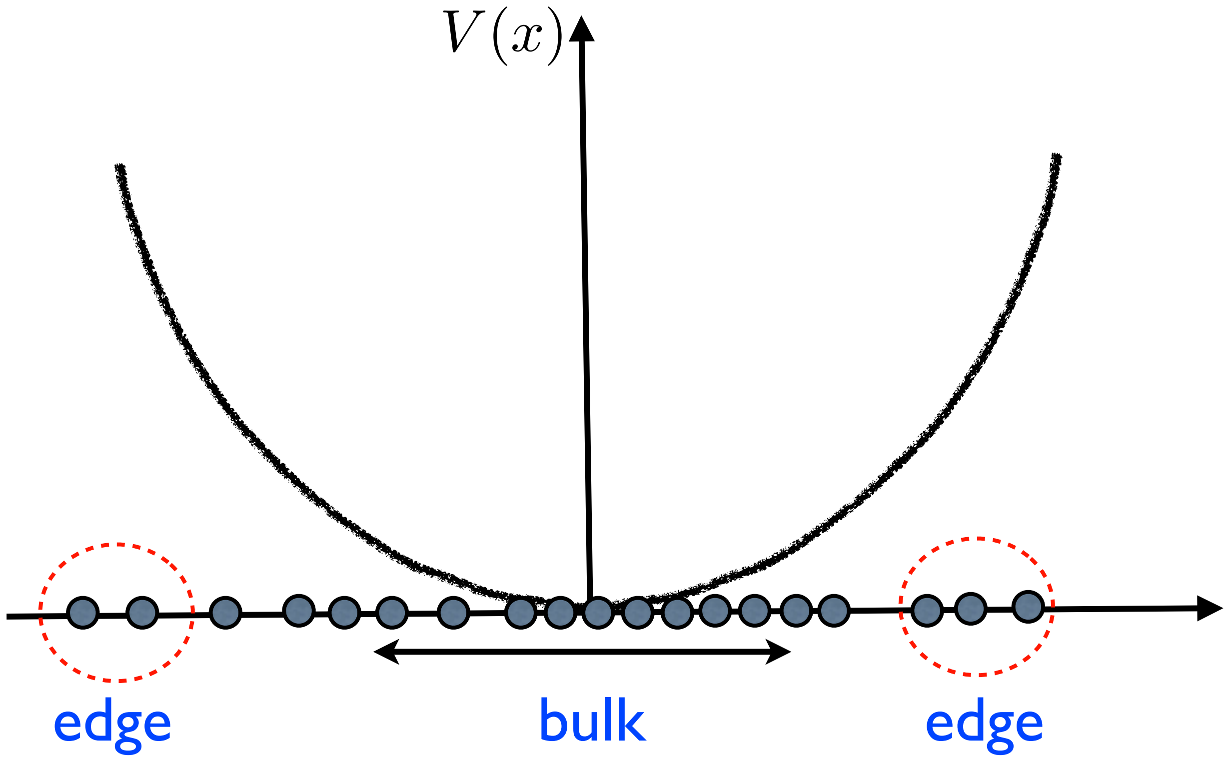


- bulk: traditional many-body physics (translationally invariant system)

  «The uniform electron gas, the traditional starting point for density-based many-body theories of inhomogeneous systems, is inappropriate near electronic edges.»

  W. Kohn, A. E. Mattsson, PRL 1998

Ultra-cold atoms in confining potentials



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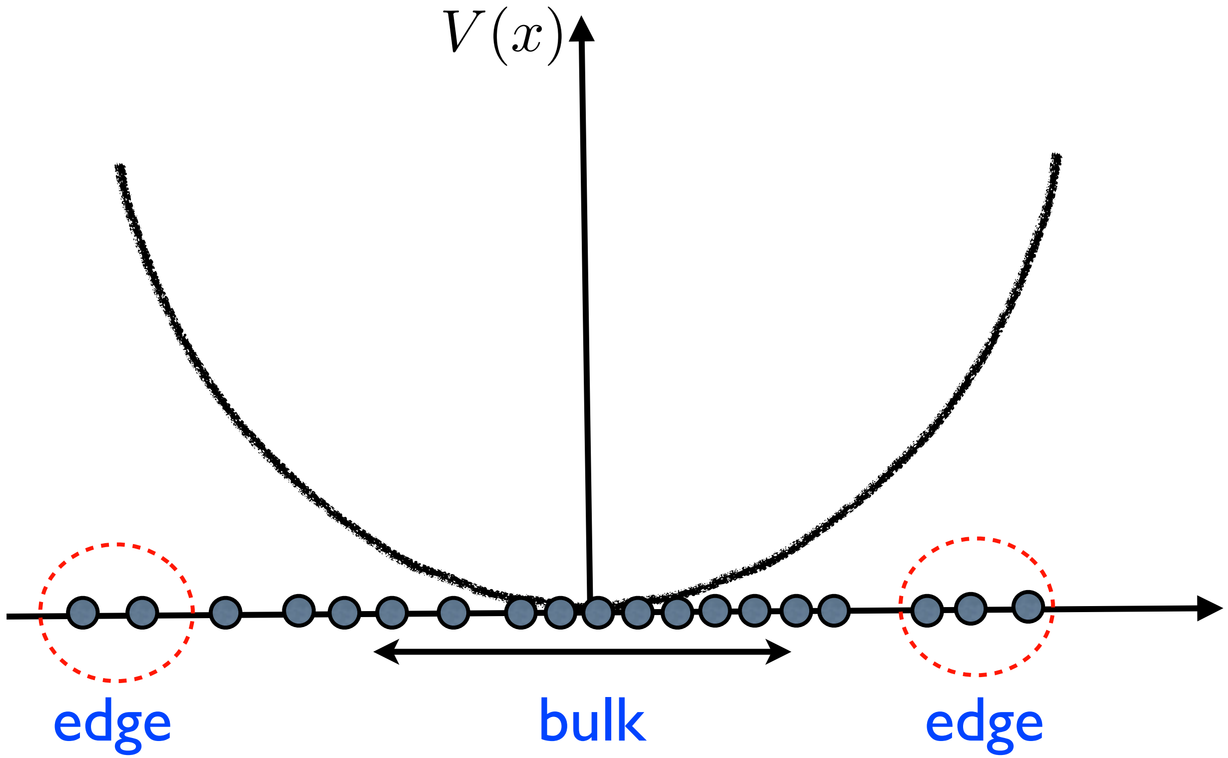
Our work: random matrix theory is the ideal tool to study these edge properties

Ultra-cold atoms in confining potentials

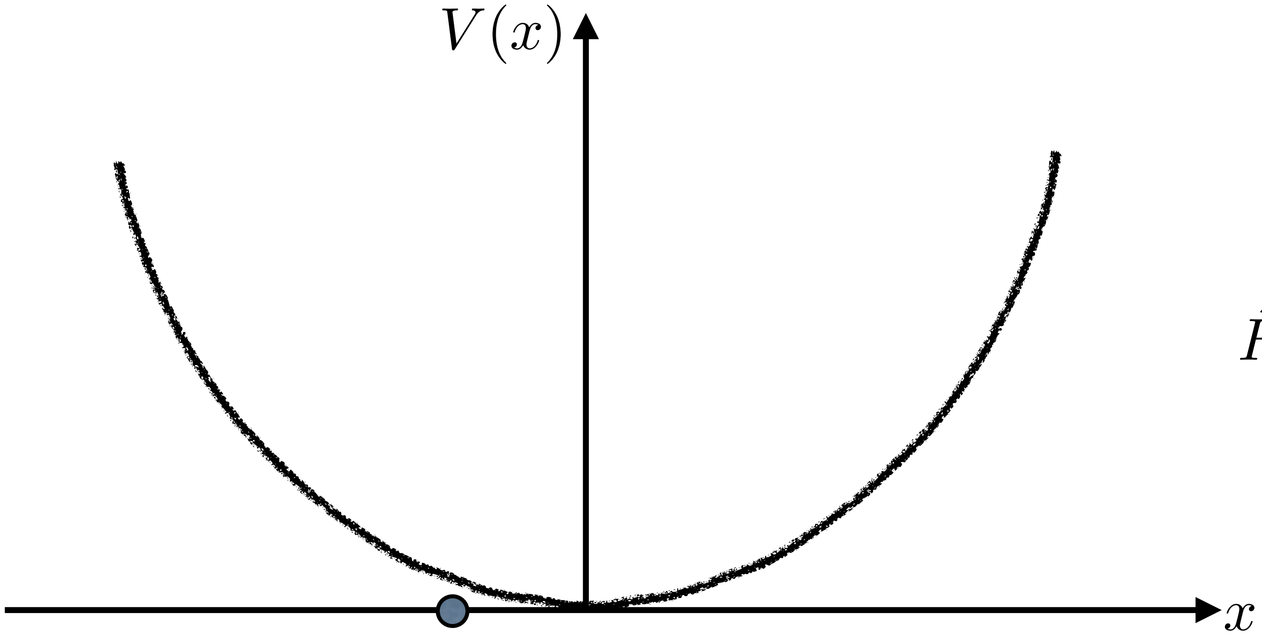


- bulk: traditional many-body physics (translationally invariant system)
- edge: new physics induced by confinement $\Rightarrow$ universal edge properties

Our work: random matrix theory is the ideal tool to study these edge properties

Connection between free fermions at T=0 and RMT

- A single quantum particle in a harmonic potential



$$V(x) = \frac{1}{2} m\omega^2 x^2$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2} m\omega^2 x^2$$

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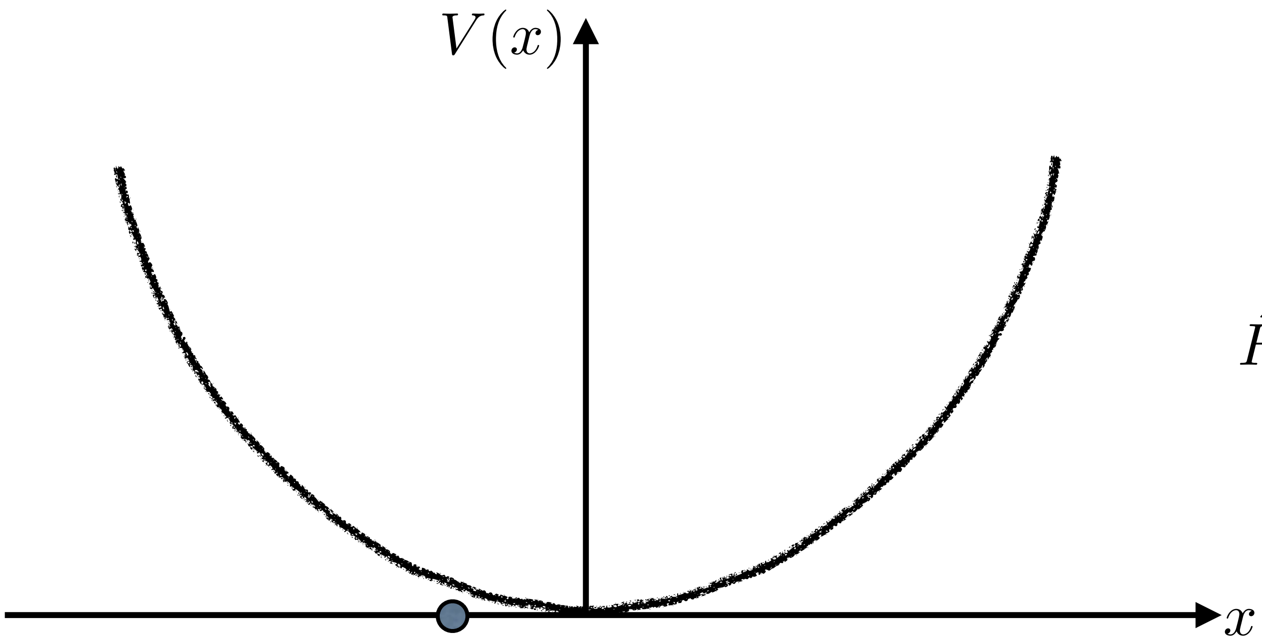

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- Single particle eigenfunctions

$$\hat{H}\,\varphi_E(x) = E\,\varphi_E(x)$$

with $\varphi_E(x \to \pm\infty) = 0$

$$\varphi_k(x) = \left[\frac{\alpha}{\sqrt{\pi} 2^k k!}\right]^{1/2} e^{-\frac{\alpha^2 x^2}{2}} H_k(\alpha x)$$

$$\epsilon_k = \hbar\omega(k + 1/2) \quad , \quad \alpha = \sqrt{m\omega/\hbar}$$

$$k \in \mathbb{N}$$

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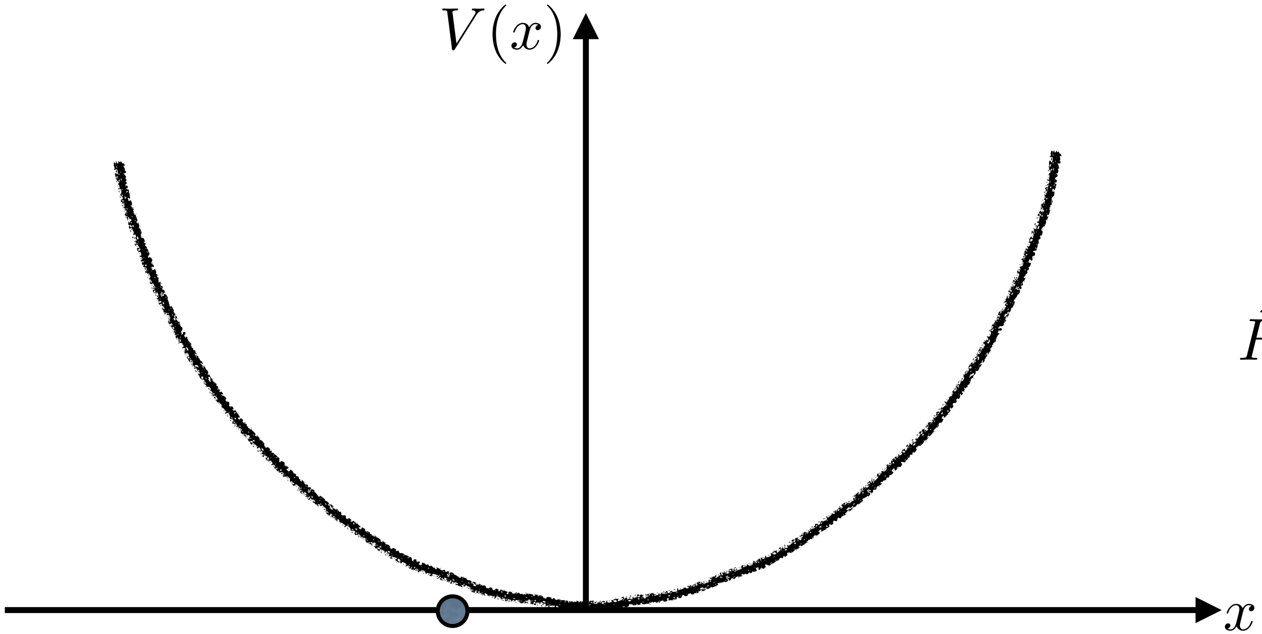

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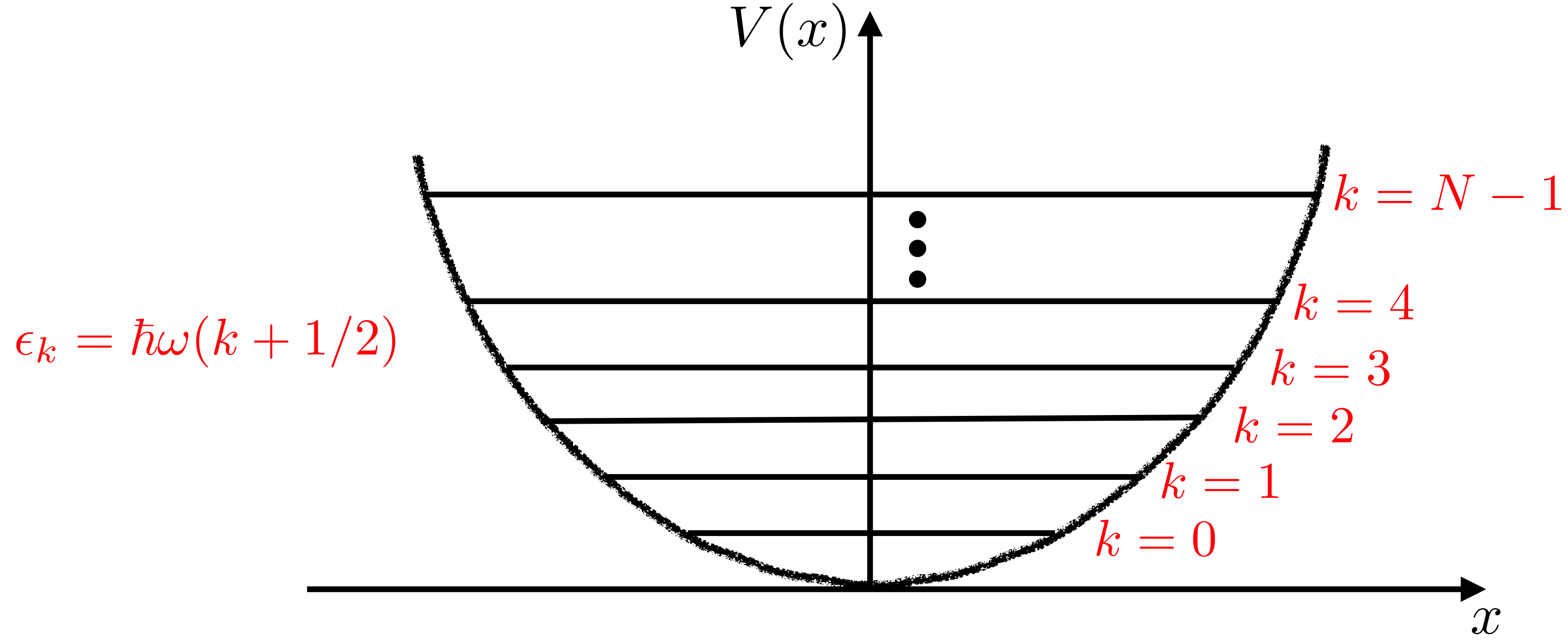
N spinless free fermions in a 1d harmonic trap at T=0



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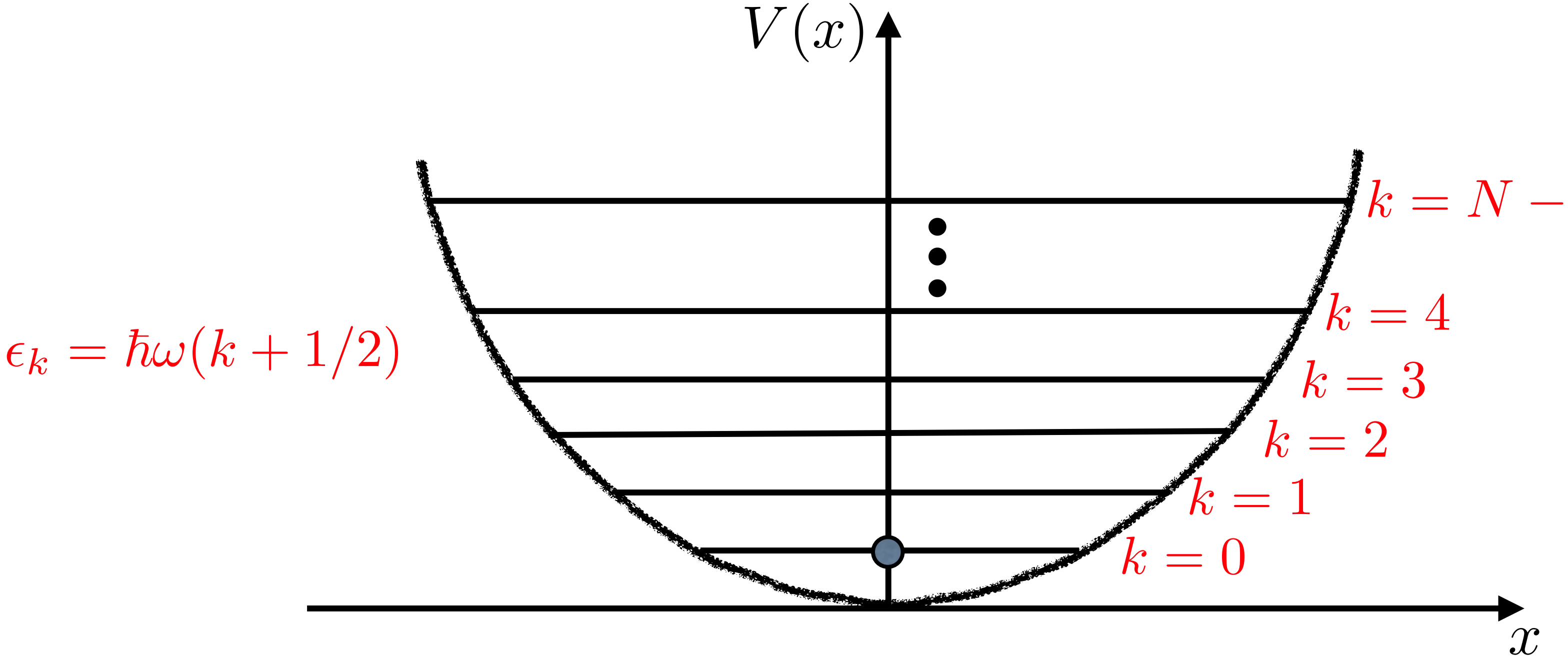

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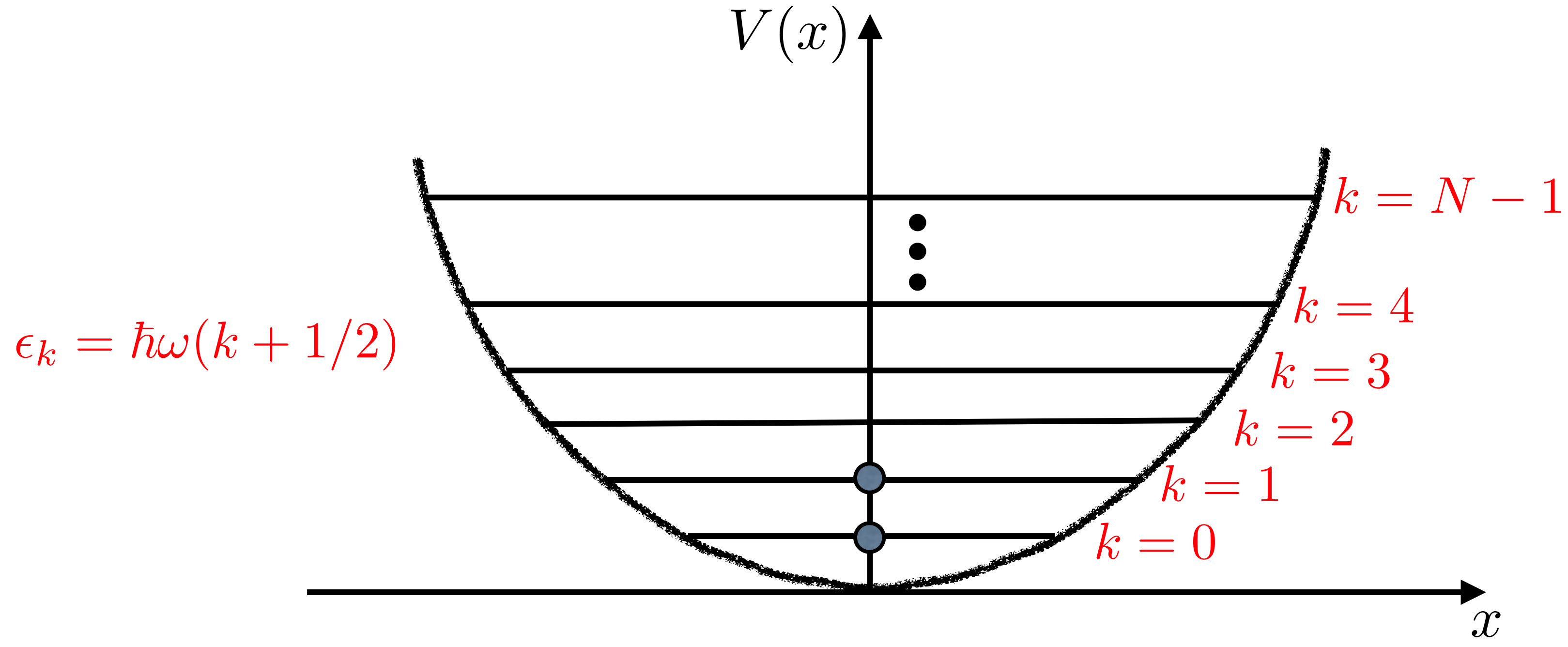

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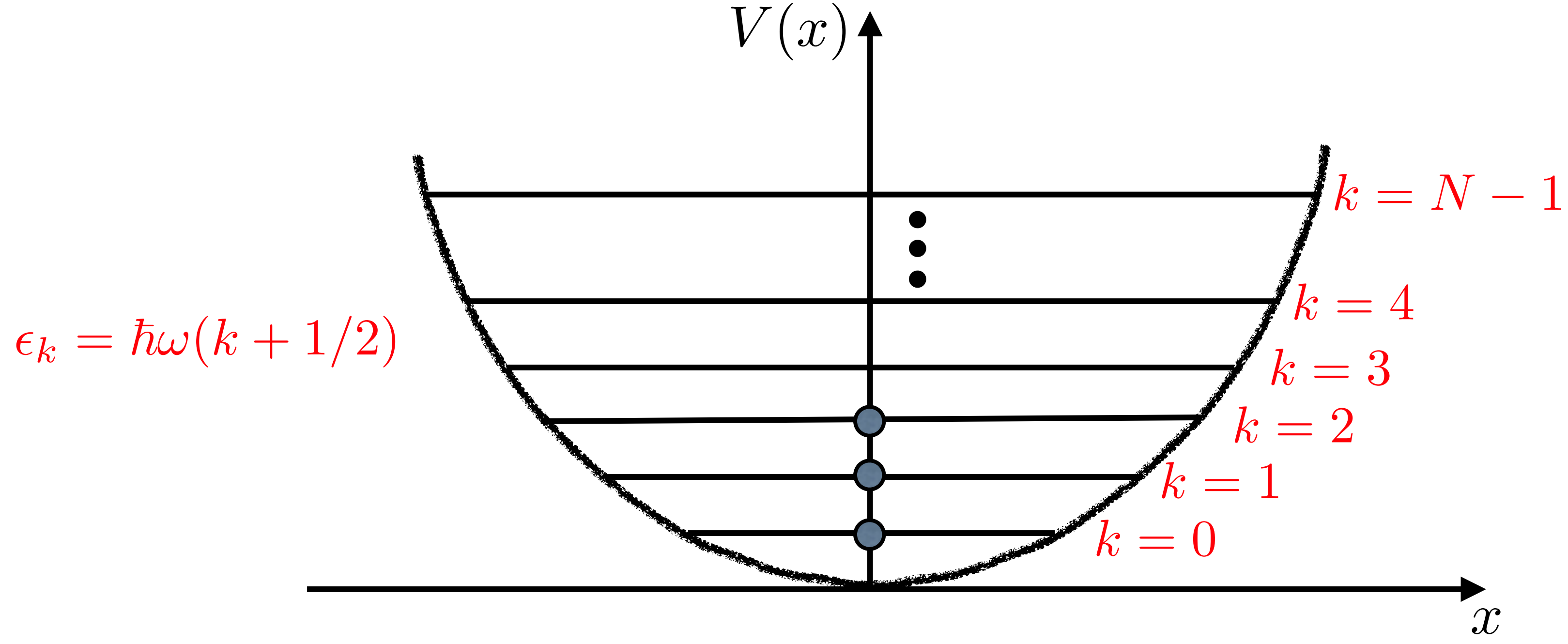

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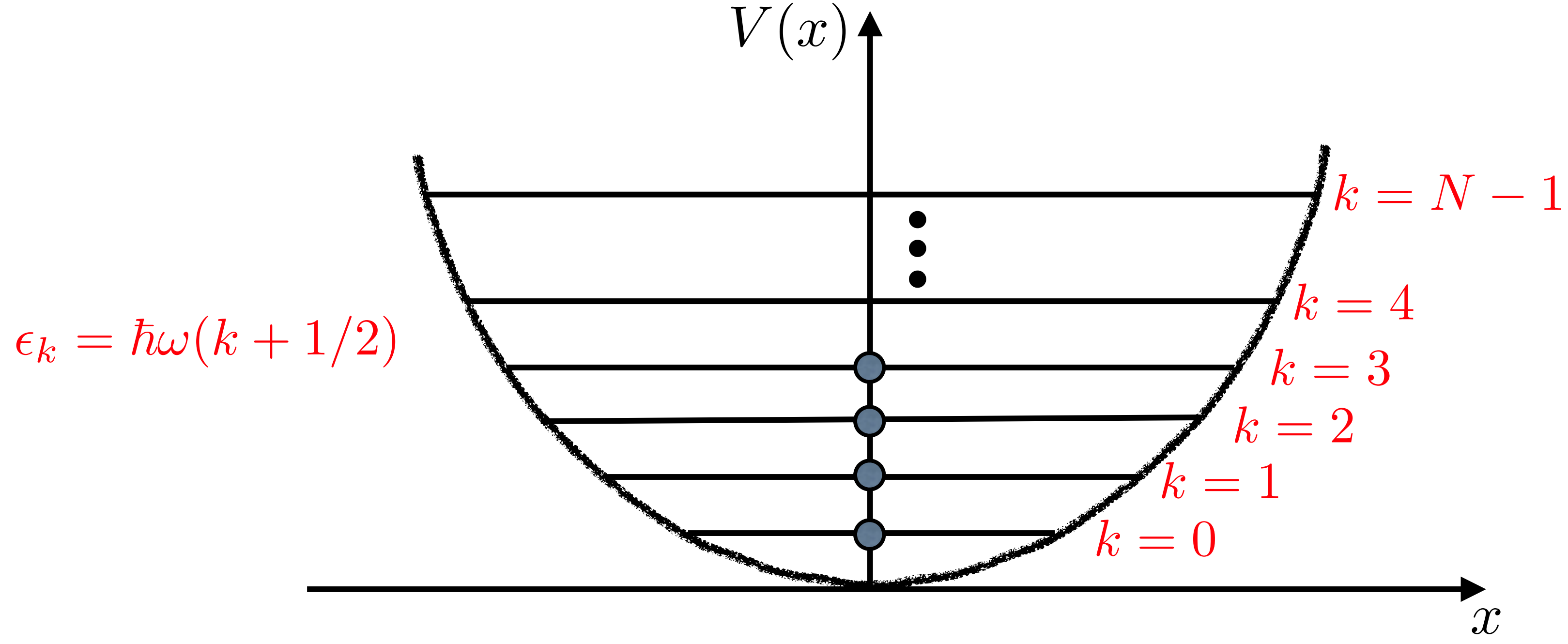

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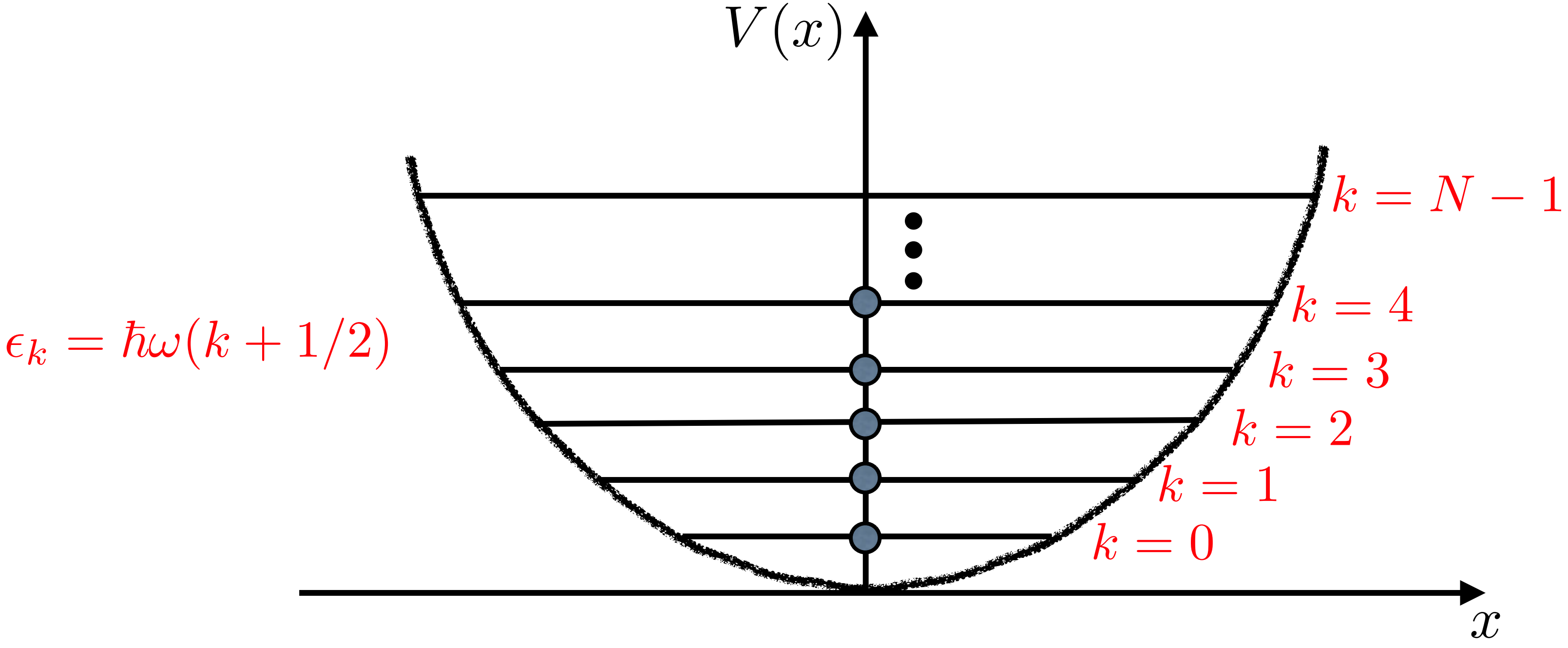

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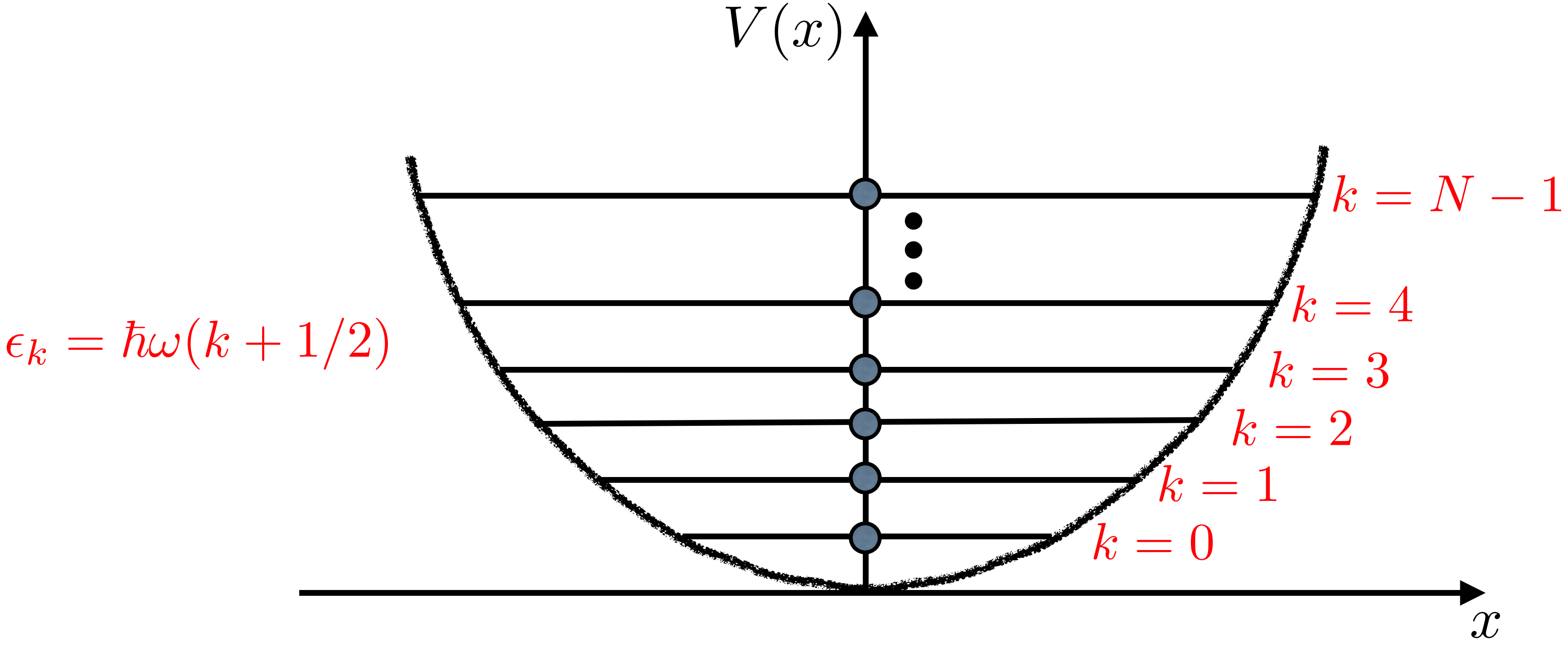

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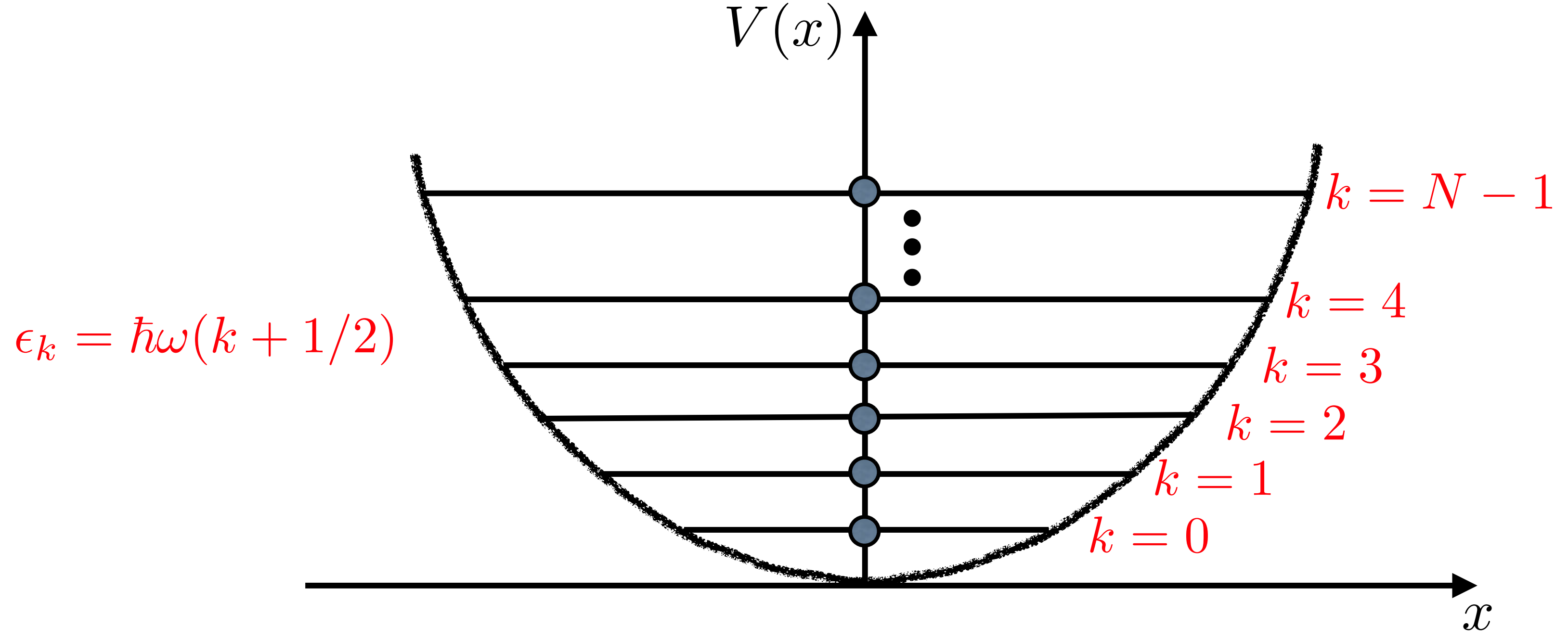

- The N-particle wave function is given by a $N \times N$ Slater determinant

$$\Psi_0(x_1, x_2, \cdots, x_N) = \frac{1}{\sqrt{N!}} \det[\varphi_i(x_j)] \qquad 0 \leq i \leq N-1$$

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$$\varphi_k(x) = \left[\frac{\alpha}{\sqrt{\pi} 2^k k!}\right]^{1/2} e^{-\frac{\alpha^2 x^2}{2}} H_k(\alpha x)$$

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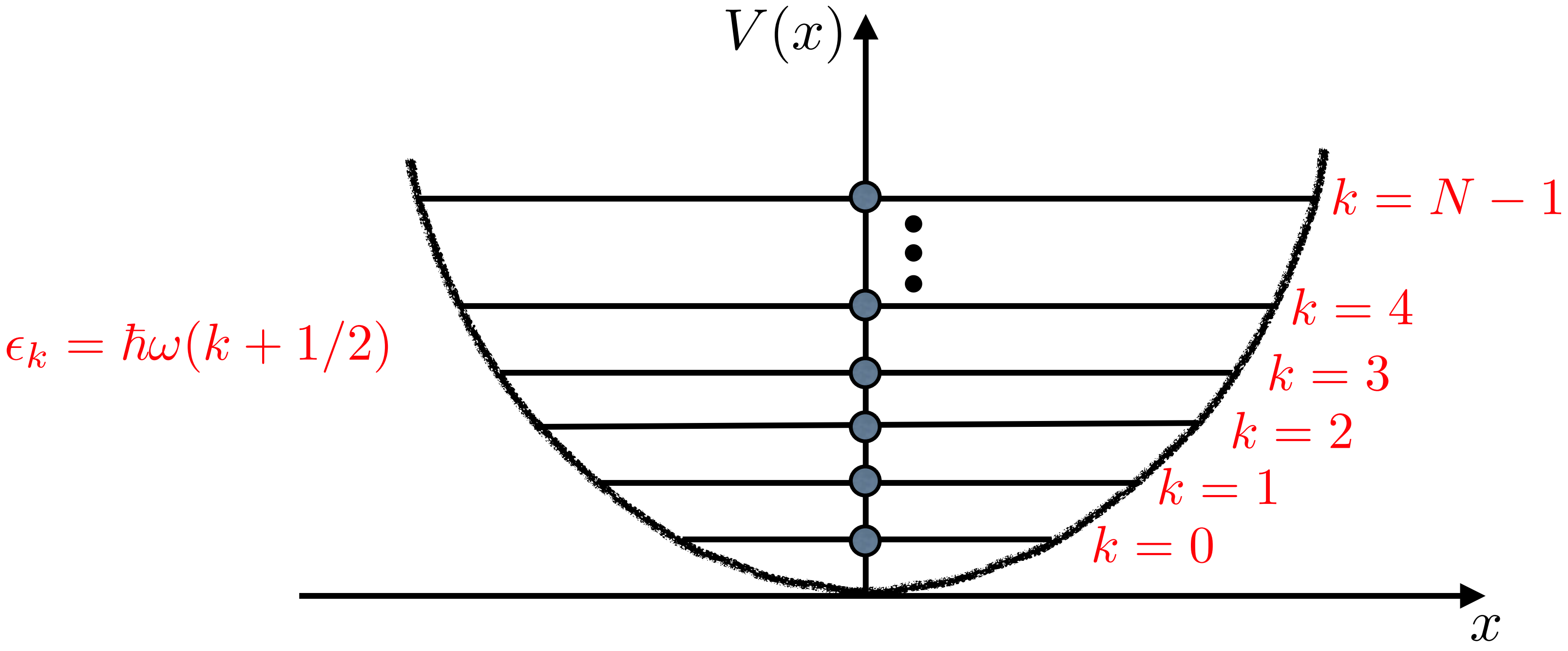

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Ground state energy $E_0 = \sum_{k=0}^{N-1} \epsilon_k = \frac{N^2}{2}$

Connection between free fermions at T=0 and RMT

- Ground-state wave function

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Hermite polynomial of degree i

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- Probability density function (PDF) of the positions $x_i' s$

$$|\Psi_0(x_1, \cdots, x_N)|^2 = \frac{1}{z_N(\alpha)} \prod_{i<j} (x_i - x_j)^2 e^{-\alpha^2 \sum_{i=1}^N x_i^2}$$

Fermions in a harmonic well at T=0 and RMT

- Squared many-body wave function (T=0 quantum probability) for fermions

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- Let J be a $N\times N$ random Hermitian matrix with Gaussian (complex) entries. The PDF of the (real) eigenvalues $\lambda_i' s$ is given by

$$P_{\text{joint}}(\lambda_1,\cdots,\lambda_N) = \frac{1}{Z_N}\prod_{i<j}(\lambda_i-\lambda_j)^2 e^{-\sum_{i=1}^N \lambda_i^2}$$

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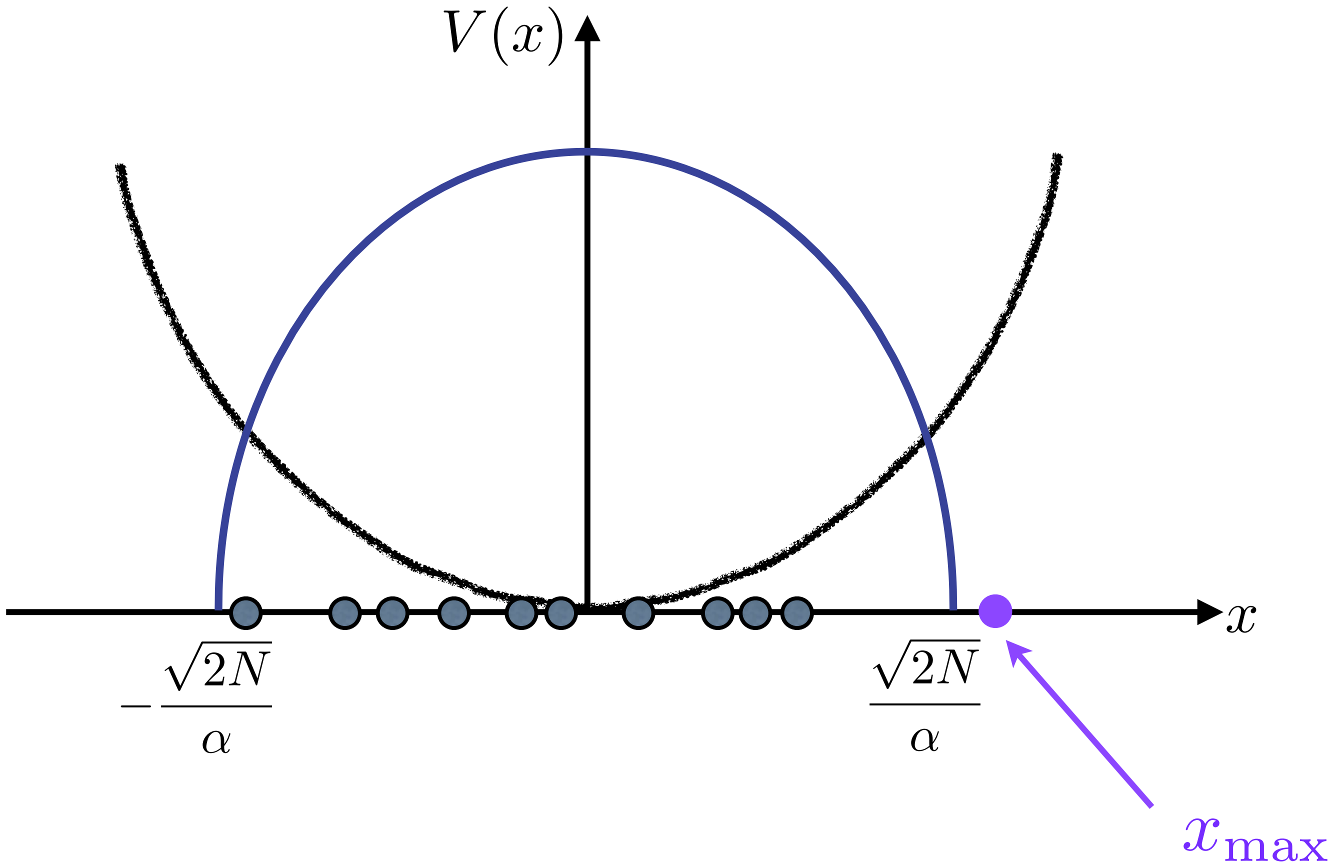
$\Rightarrow$ The positions of the free fermions behave statistically like the eigenvalues of GUE random matrices

$\Rightarrow$ The spatial properties of free fermions in a harmonic trap at T=0 can directly be obtained from the known results in RMT

Eisler '13/Marino, Majumdar, G. S., Vivo '14/Calabrese, Le Doussal, Majumdar '15

Position of the rightmost fermion at T=0



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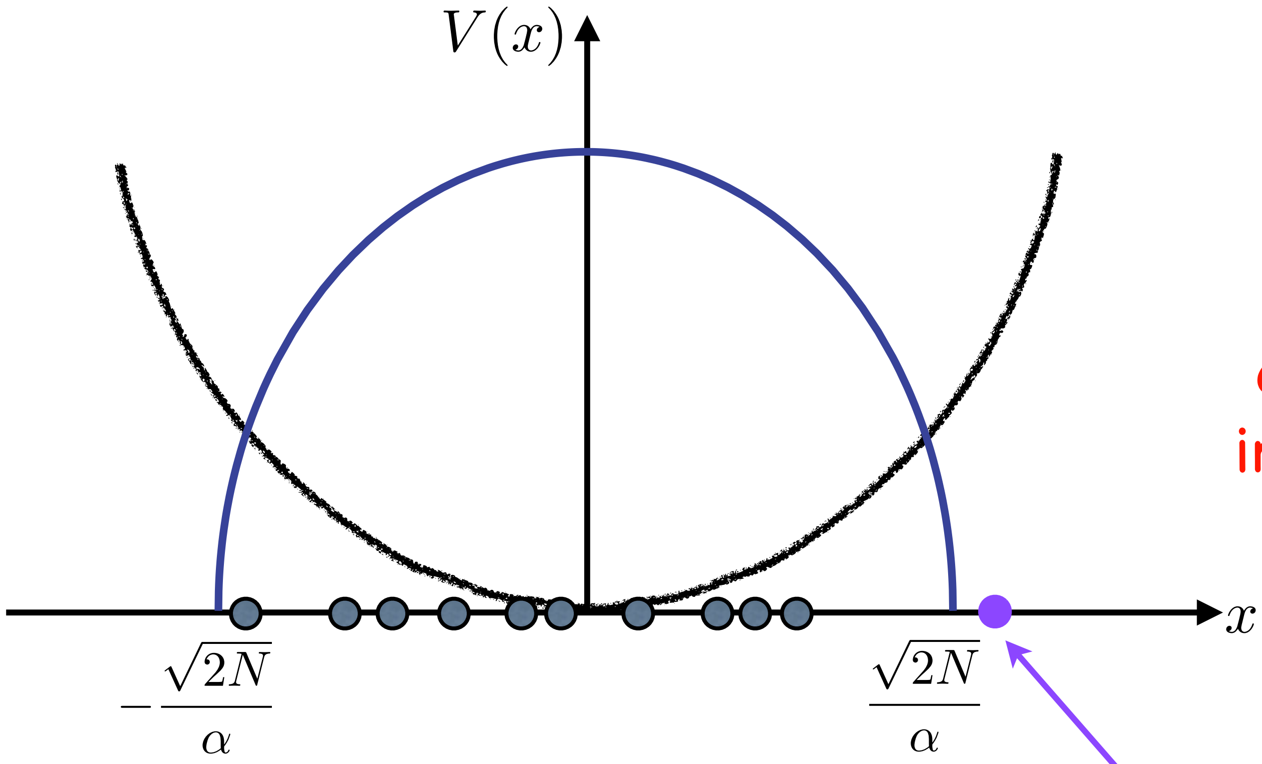

largest eigenvalue
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from the connection with RMT:

$$x_{\max} \stackrel{d}{=} \frac{\lambda_{\max}}{\alpha}$$

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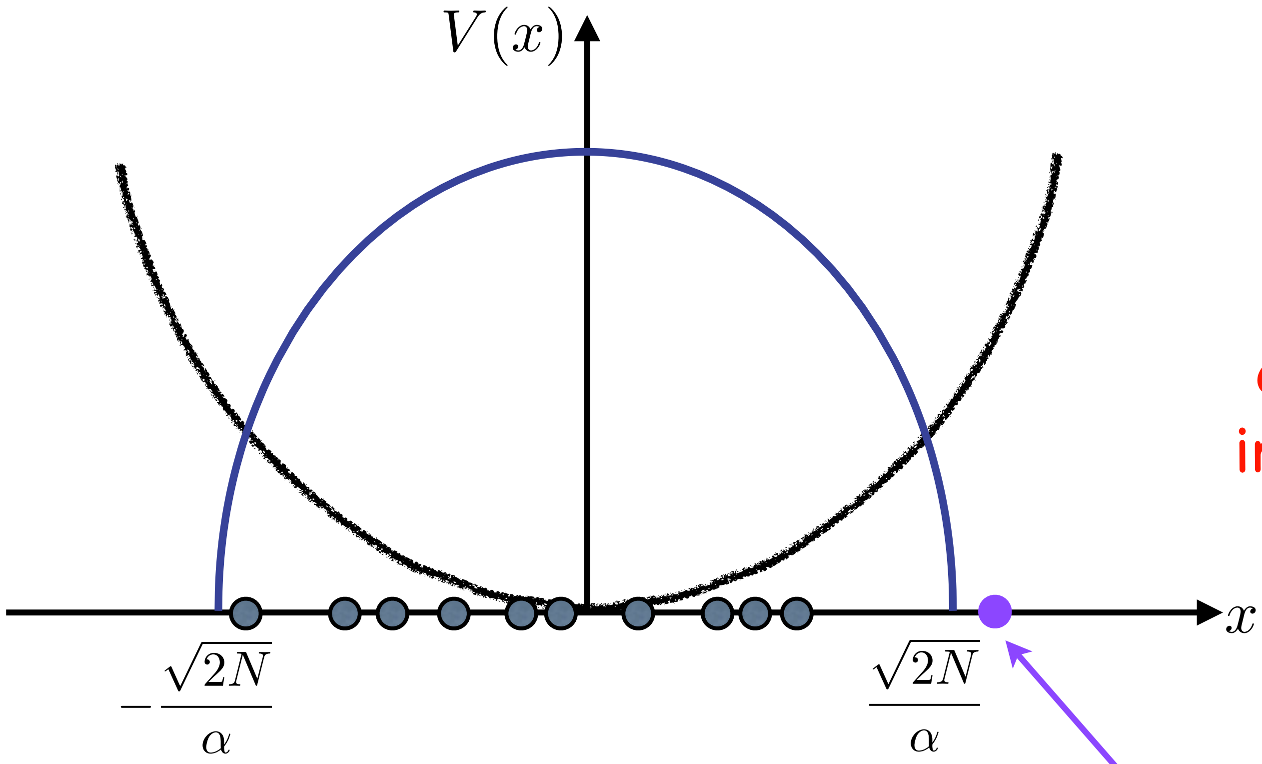

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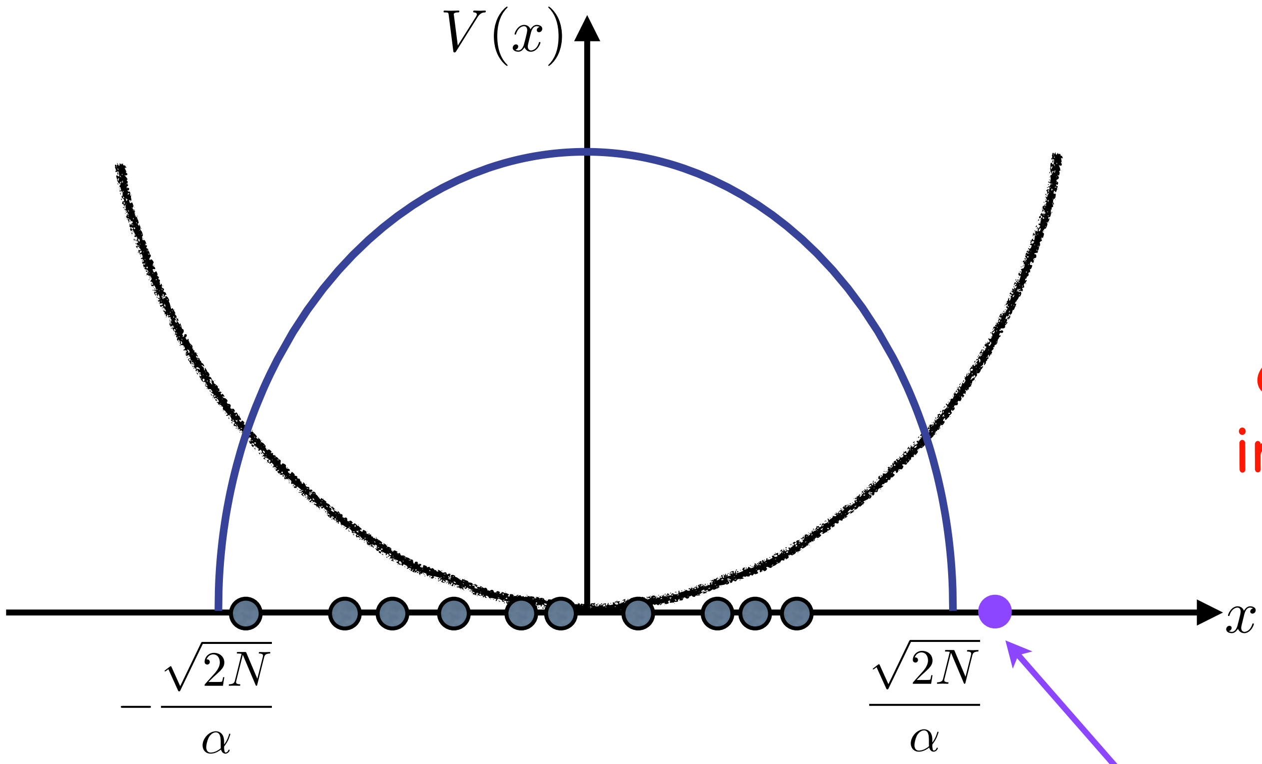

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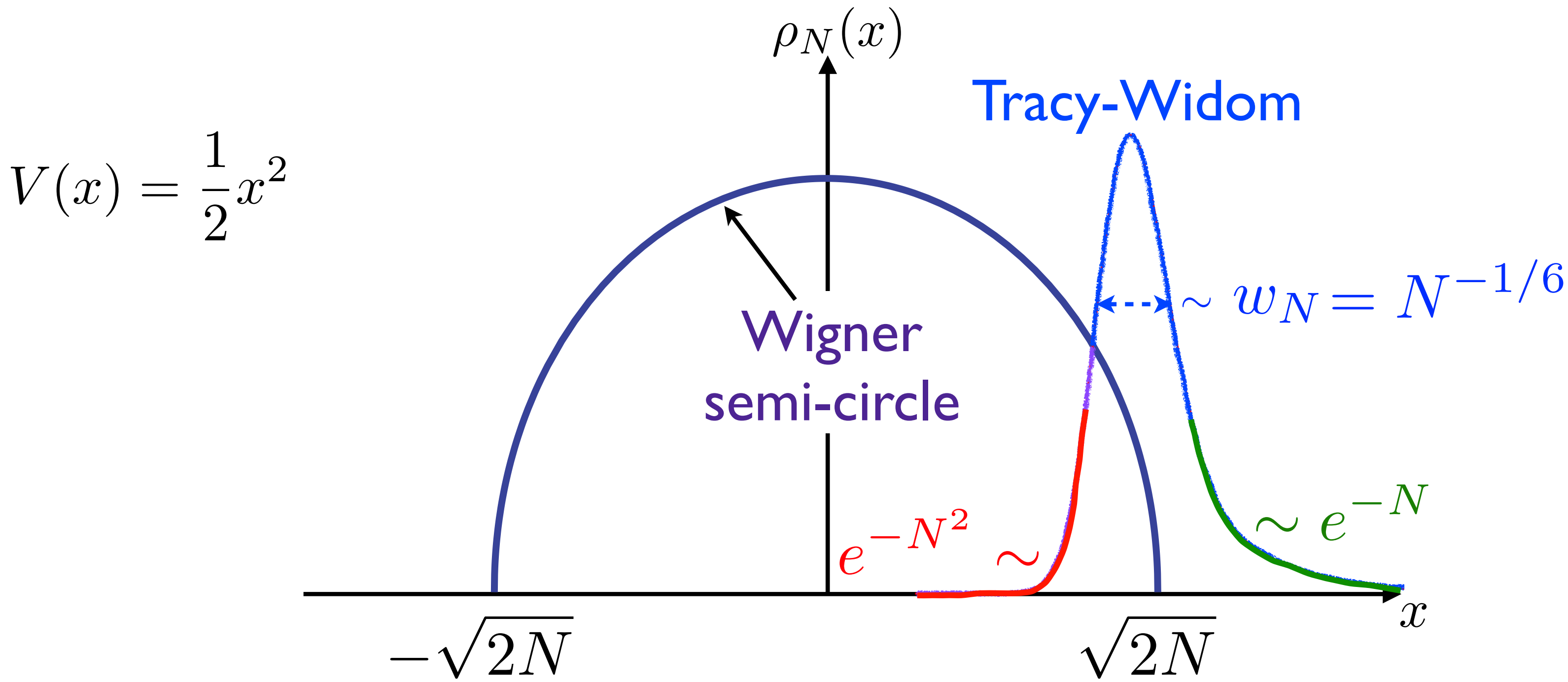
⇒ typical fluctuations of $x_{\max}(T=0)$ are governed by the Tracy-Widom distribution for GUE

⇒ large deviations away from $\sqrt{\frac{2N}{\alpha}}$ are also know in GUE

Large deviations of the position of the rightmost fermion



$$\Pr(x_{\max} \le M) \sim \begin{cases} e^{-N^2 \Phi_-(M/\sqrt{N})}\ , \text{ for } \ 0 < (\sqrt{2N} - M) = O(\sqrt{N}) & \text{left} \\ \mathcal{F}_2\left(w_N\,(M - \sqrt{2})\right)\ , \text{ for } \ M - \sqrt{2N} = O(w_N) & \text{Tracy Widom} \\ 1 - e^{-N\Phi_+(M/\sqrt{N})}\ , \text{ for } \ 0 < (M - \sqrt{2N}) = O(\sqrt{N})\ , & \text{right} \end{cases}$$

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- Smooth matching between the three regimes

Large deviations of the position of the rightmost fermion

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- Universal scenario for smooth one-dimensional potential, e.g. $V(x) \sim x^p$

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- Universal scenario for smooth one-dimensional potential, e.g. $V(x) \sim x^p$

⟹ central part is universal (Tracy-Widom)

Large deviations of the position of the rightmost fermion

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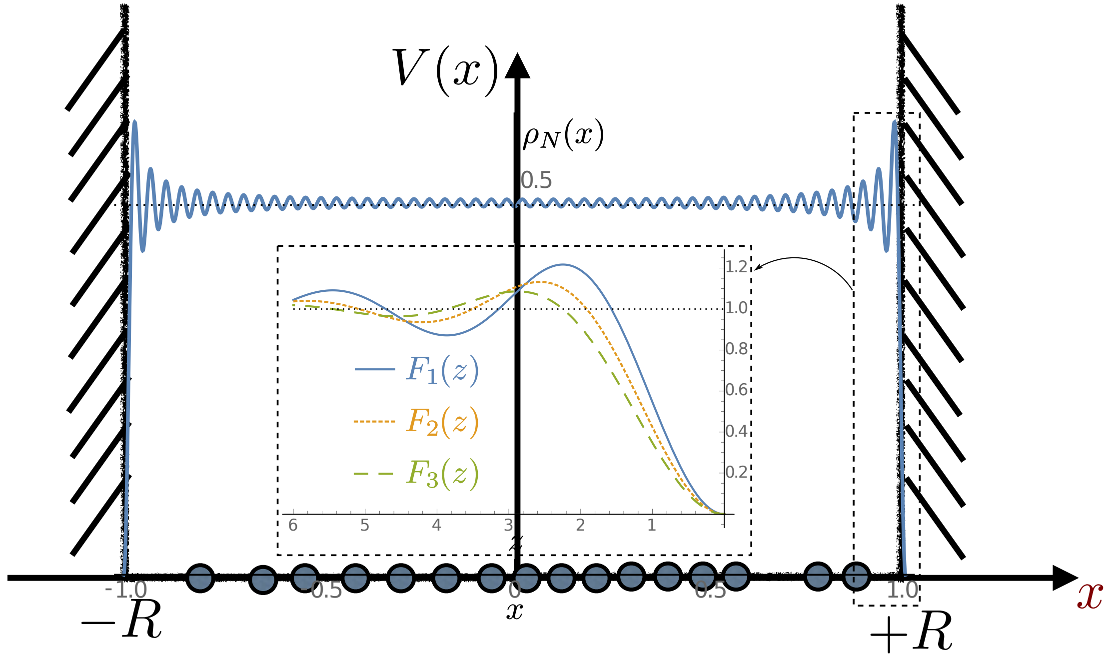
What about other universality classes ?

Fermions in a hard box at T=0 and RMT

$$V(x) = \begin{cases} 0\,, & |x| \leq R \\ +\infty\,, & |x| > R \end{cases}$$



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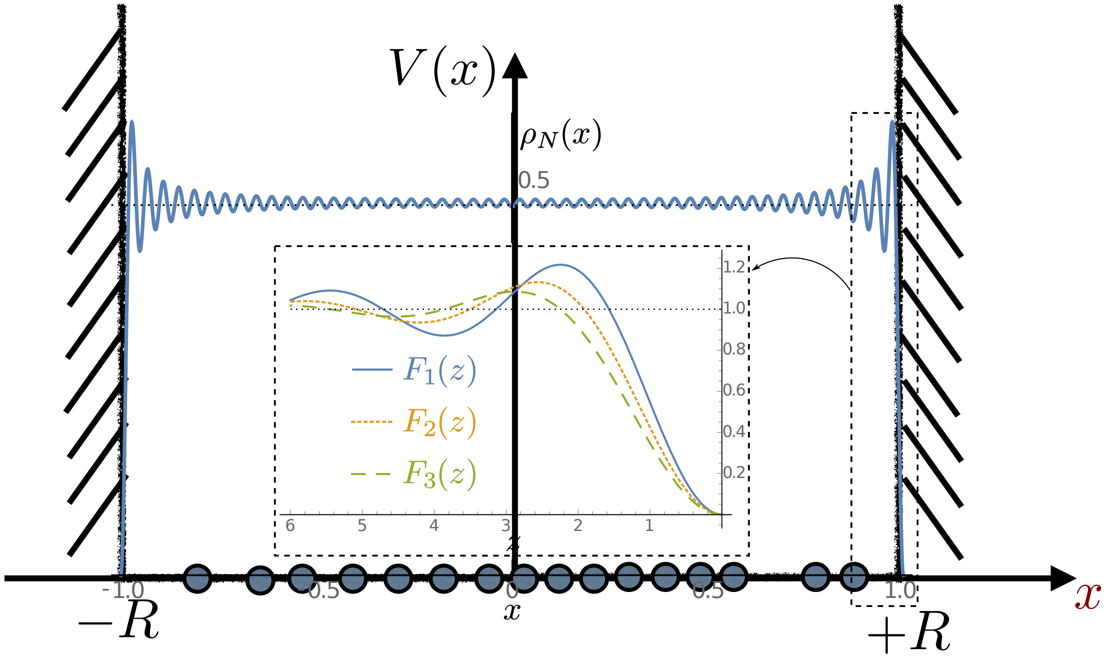

- Squared many-body wave function (T=0 quantum probability) for fermions

$$|\Psi_0(x_1, x_2, \cdots, x_N)|^2 = \frac{1}{z_N(R)} \prod_{i=1}^{N} (1 - v_i^2) \prod_{j<k}^{N} |v_j - v_k|^2 \,, \;\; v_j = \sin \frac{\pi x_j}{2R}$$

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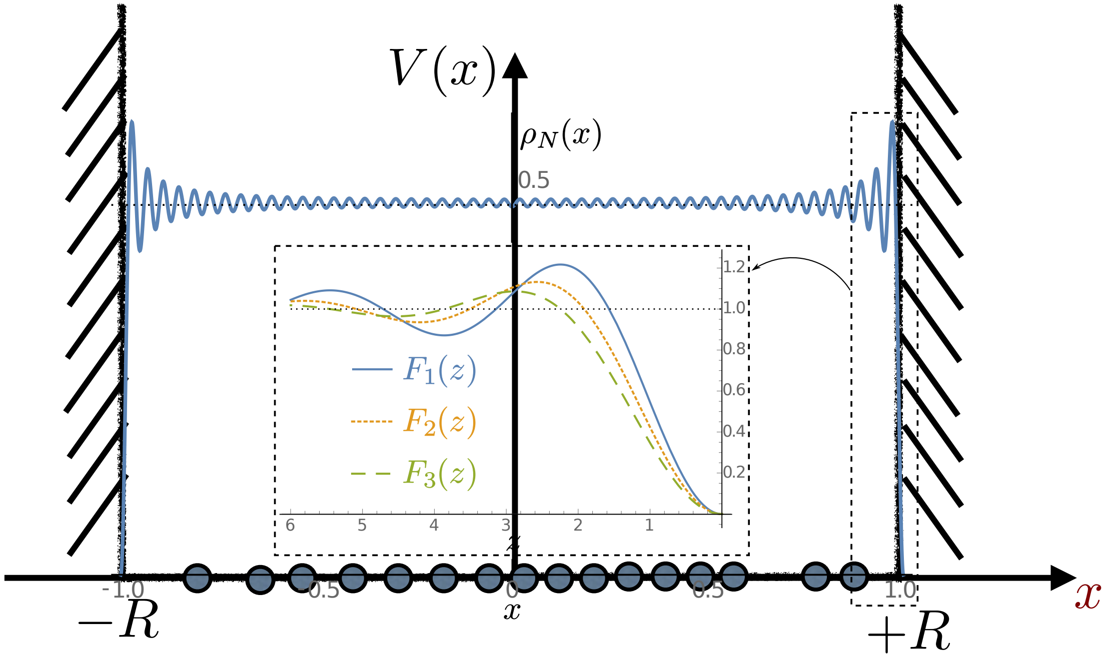

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⟹ identical to the Jacobi Unitary Ensemble in Random Matrix Theory

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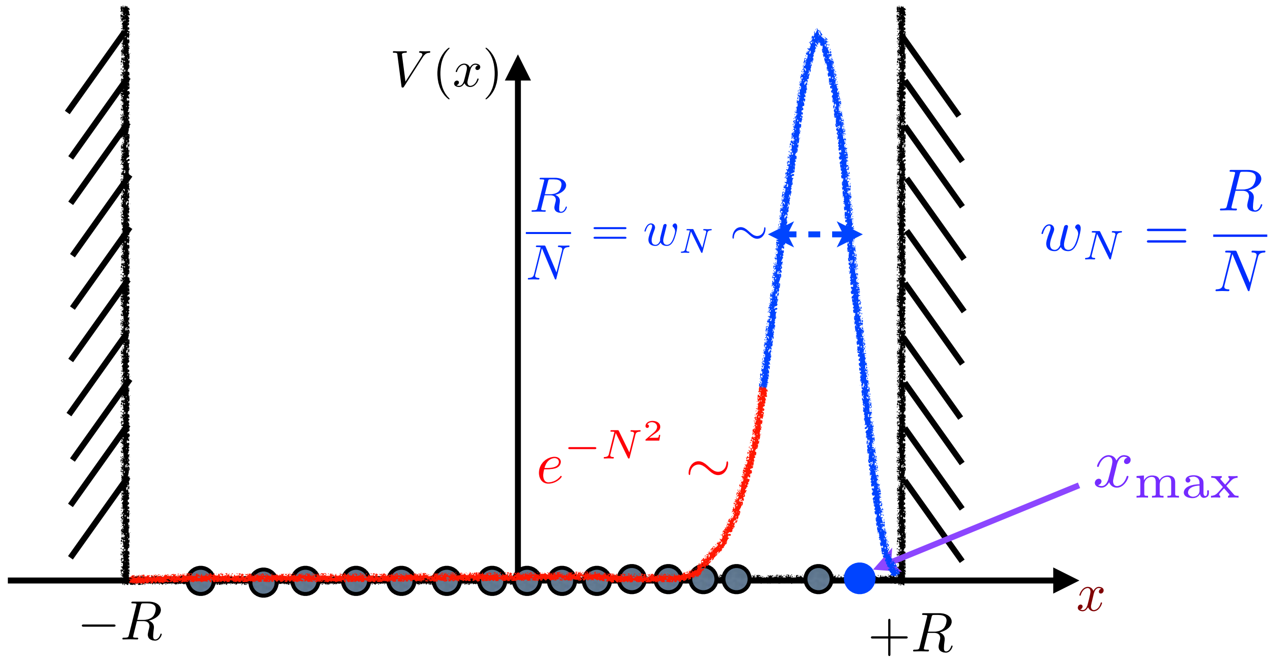
Position of the rightmost fermion at T=0



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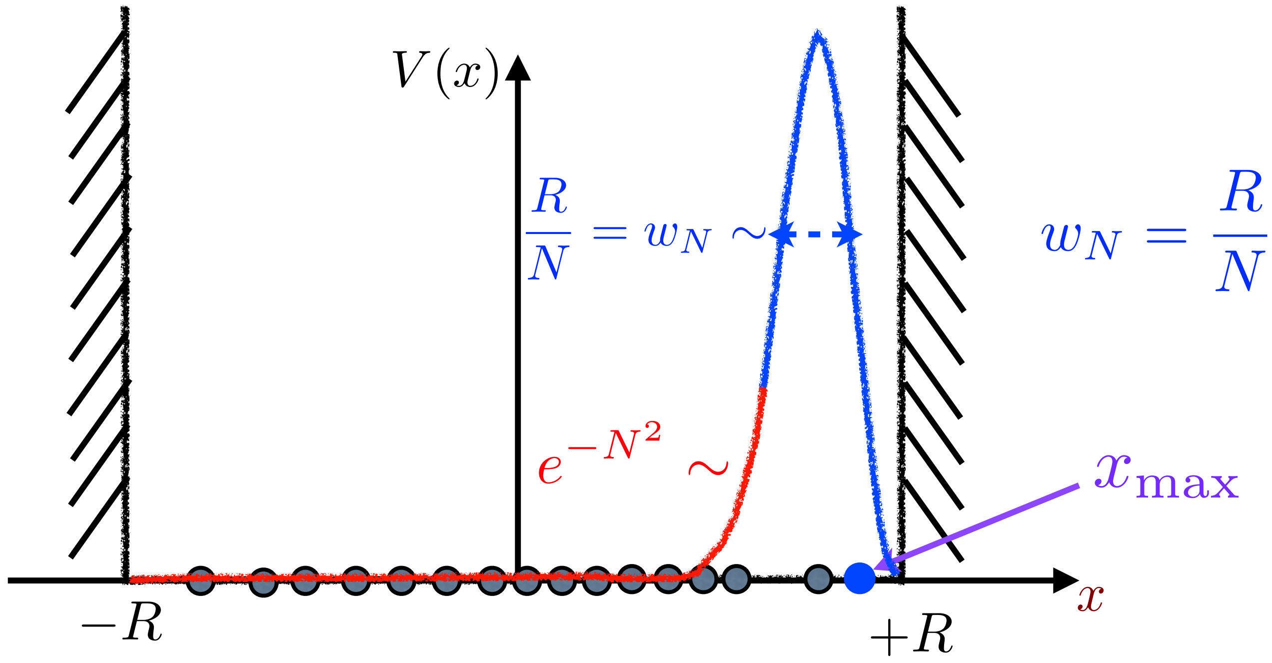

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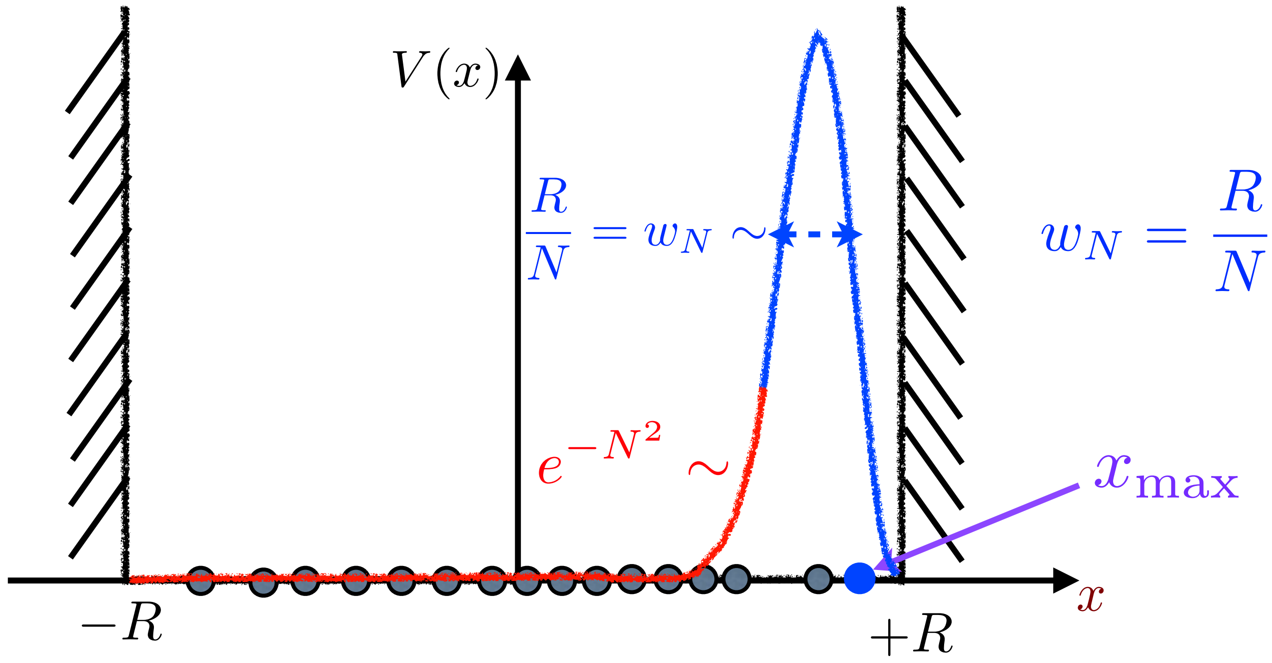

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$$\Phi_-(x) = \ln\left(\frac{2}{1+\sin\left(\frac{\pi}{2}x\right)}\right), \quad -1 \leq x \leq 1$$

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What happens in $d > 1$?

Fermions in a d-dimensional spherical hard box

- N-body quantum Hamiltonian

$$\mathcal{H}_N = \sum_{j=1}^{N} H_j \ , \quad \text{where} \qquad H_j = -\frac{\hbar^2}{2m}\Delta_{\mathbf{x}_j} + V(\mathbf{x}_j)$$

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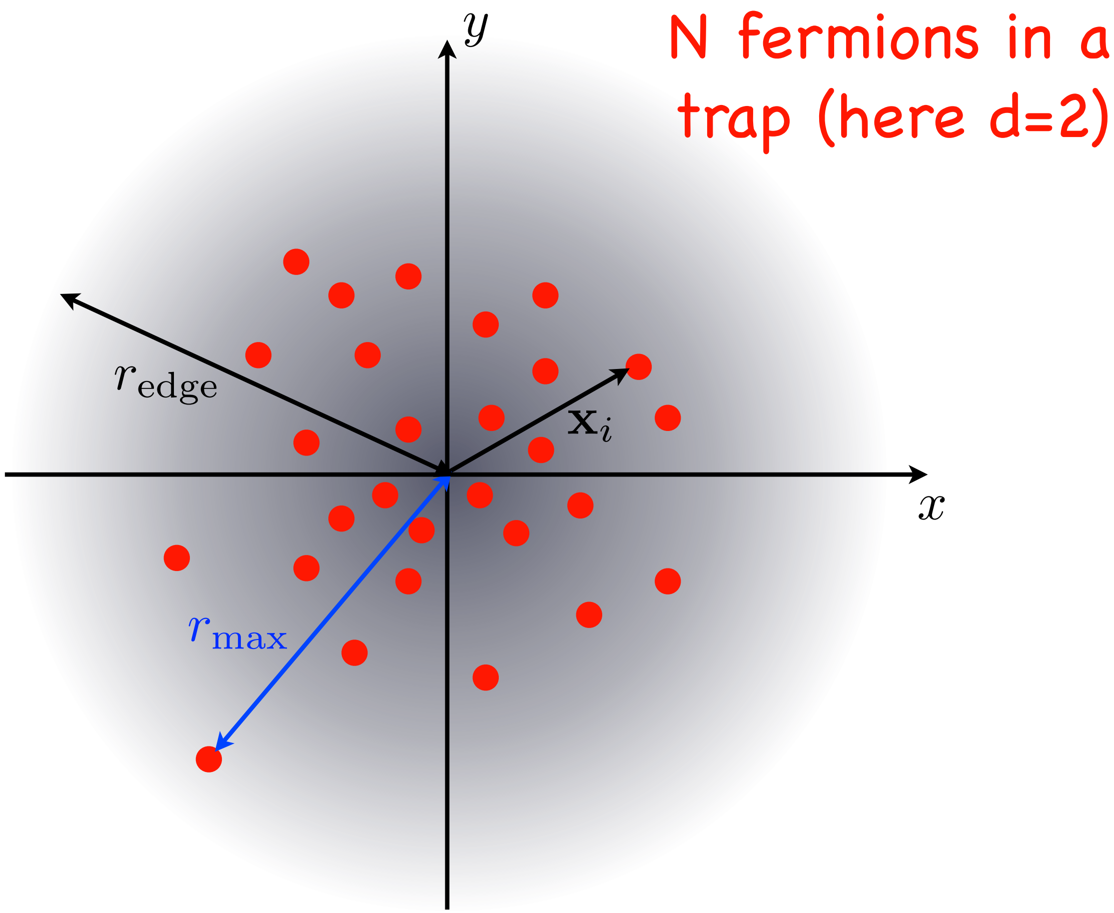
- Typical scale of correlations is $w_N = 1/k_F \sim N^{-1/d}$

Fermi wave vector

Radial distance of the farthest fermion in d>1



$$r_{\max} = \max(r_1, r_2, \ldots, r_N) \quad \text{where} \quad r_i^2 = \mathbf{x_i} \cdot \mathbf{x_i}$$

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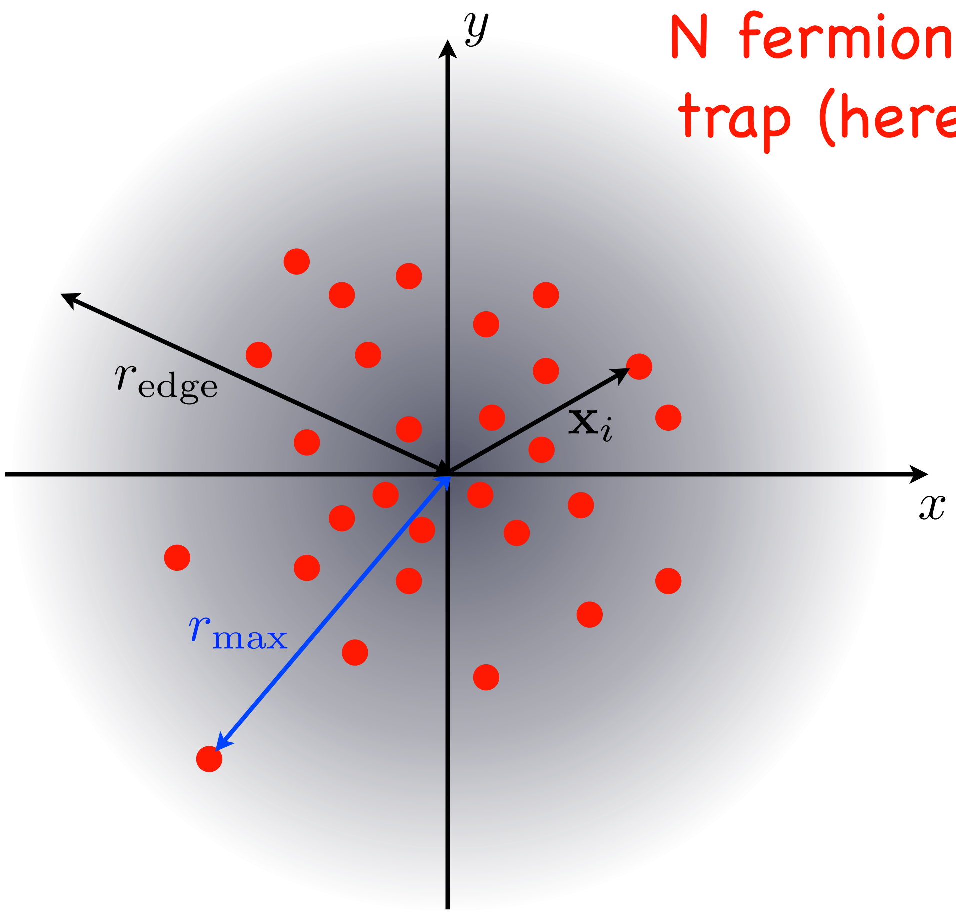

N fermions in a trap (here d=2)

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box size: $R = 1$

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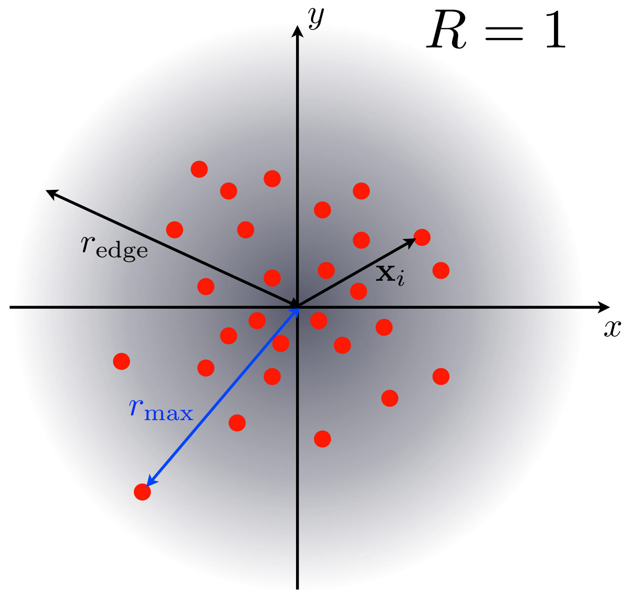

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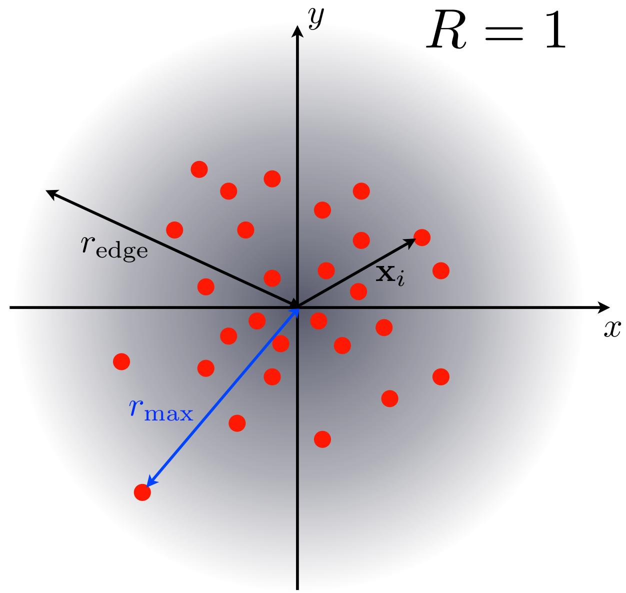
$\Rightarrow$ special case of a Weibull distribution



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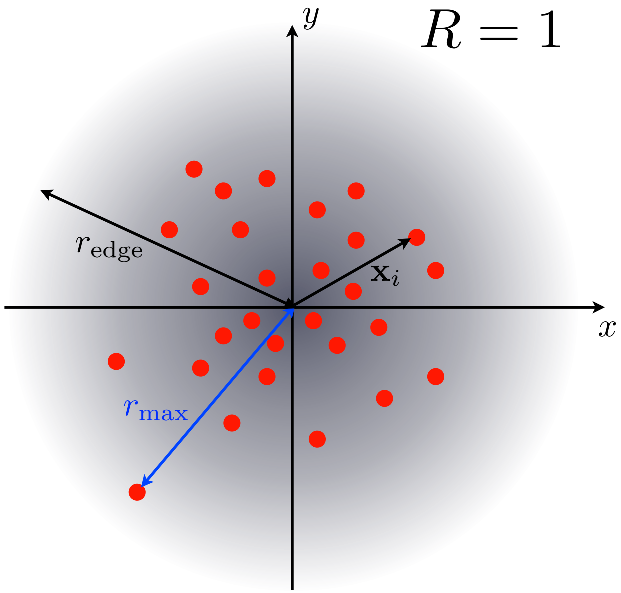

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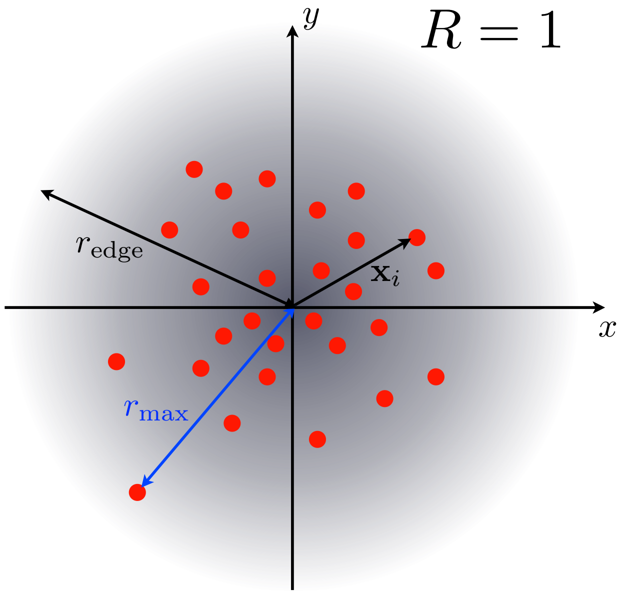

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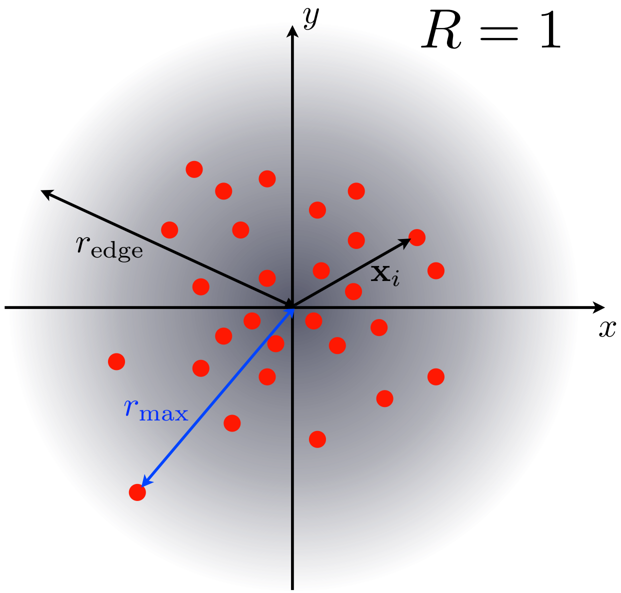

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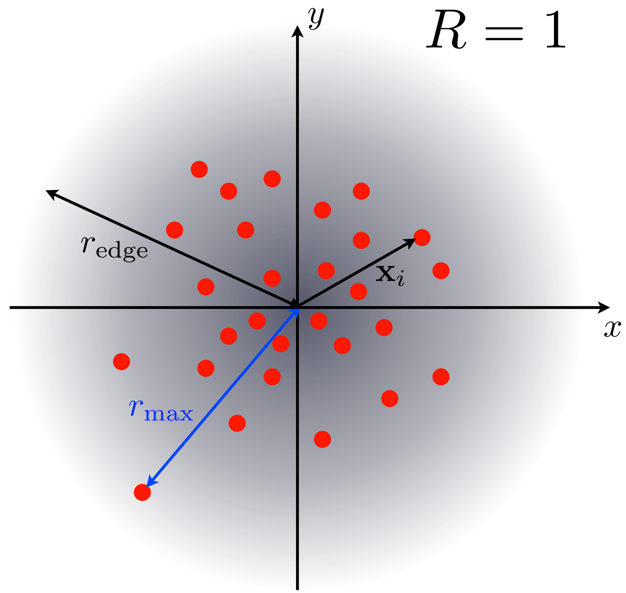

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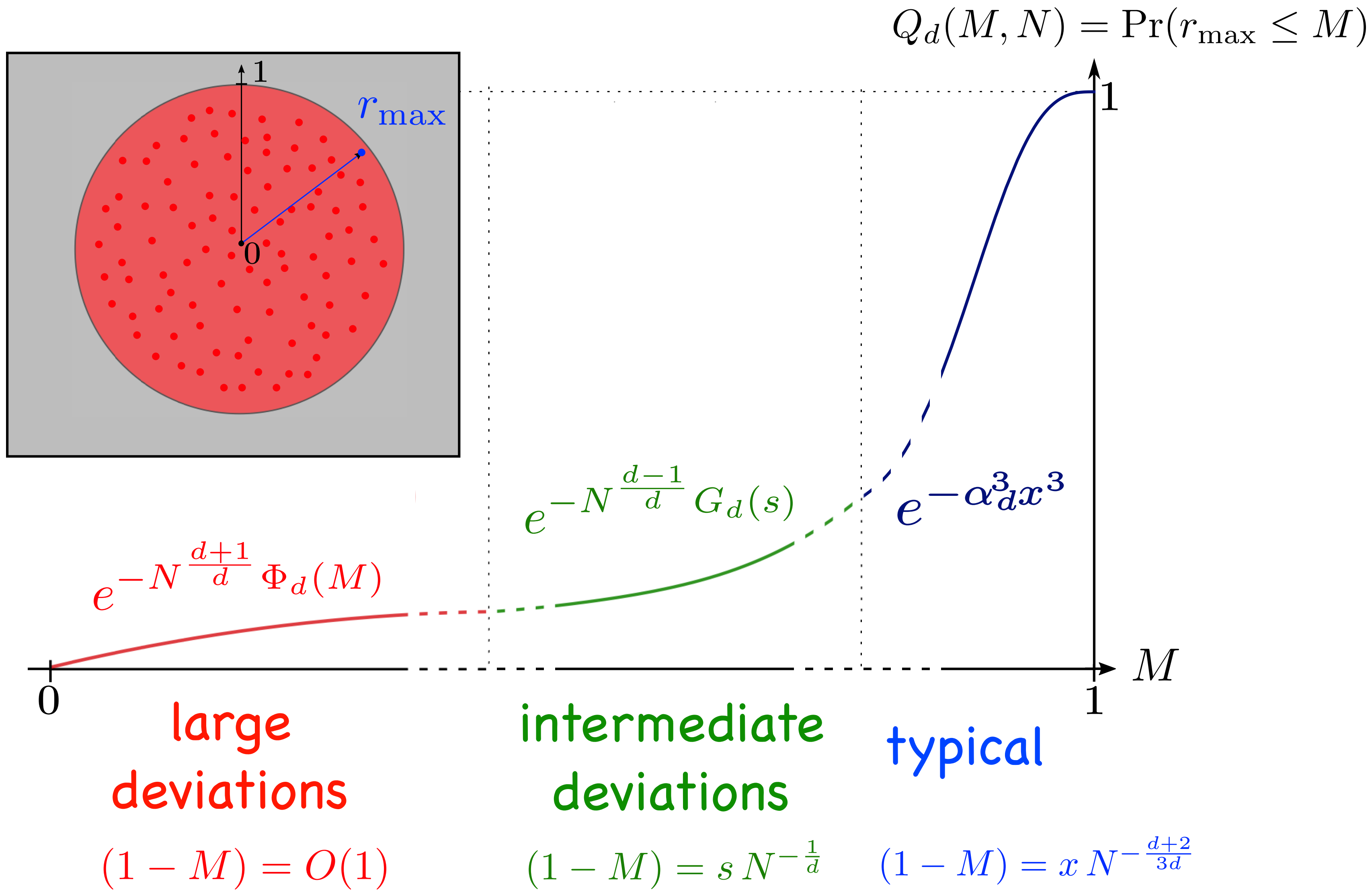

Sketch of the derivation

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D. S. Dean, P. Le Doussal, S. N. Majumdar, G. S., PRA 94, 063622 (2016)

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B. Lacroix-A-Chez-Toine, P. Le Doussal, S. N. Majumdar, G. S., arXiv:1706.03598

Free fermions in a spherically symmetric potential (T=0)

- Single particle Hamiltonian

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Free fermions in a d-dimensional trap (T=0)

- Quantum probability (i.e., modulus squared wave function)

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$\Rightarrow$ free fermions in d-dimensions form a d-dimensional determinantal process

A determinantal expression for the CDF of $r_{\max}$

- Ground state wave function

$$\Psi_0(\mathbf{x}_1, \cdots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \det_{1 \leq i,j \leq N} [\psi_{\mathbf{k}_i}(\mathbf{x}_j)]$$

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$$I_M(\mathbf{x}) = \begin{cases} 1\ , & |\mathbf{x}| \ge M \\ 0\ , & |\mathbf{x}| < M \end{cases}$$

indicator function

average in the ground state

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$$Q_d(M, N) = \frac{1}{N!} \int d\mathbf{x}_1 \ldots \int d\mathbf{x}_N \det_{1 \le i,j \le N} [\psi^*_{\mathbf{k}_i}(\mathbf{x}_j)] \det_{1 \le i,j \le N} [\psi_{\mathbf{k}_i}(\mathbf{x}_j)] \prod_{i=1}^{N} (1 - I_M(\mathbf{x}_i))$$

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- Using Cauchy-Binet formula

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$\Longrightarrow$ use spherical coordinates $(r, \boldsymbol{\theta})$

Single particle eigenstates in spherical coordinates

$$\hat{H} = -\frac{1}{2}\nabla^2_{\mathbf{x}} + V(r) \quad \text{where} \quad V(r) = \begin{cases} 0 & , \ r \leq R \\ +\infty & , \ r > R \end{cases}$$

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$$\left[-\frac{1}{2\,r^{d-1}} \frac{\partial}{\partial r} \left(r^{d-1} \frac{\partial}{\partial r} \right) - \frac{\hat{\Delta}_{\boldsymbol{\theta}}}{2\,r^2} + V(r) \right] \psi_{\mathbf{k}_i}(r, \boldsymbol{\theta}) = \epsilon_{\mathbf{k}_i}\, \psi_{\mathbf{k}_i}(r, \boldsymbol{\theta})$$

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$$\lambda = -l(l+d-2) \ , \quad l \in \mathbb{N}$$

with degeneracy $g_d(l)$

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- Note also that

$$\int d\boldsymbol{\theta}\; Y_{\mathbf{L}}(\boldsymbol{\theta}) Y_{\mathbf{L}'}(\boldsymbol{\theta}) = \delta_{\mathbf{L},\mathbf{L}'}$$

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d-dimensional spherical harmonics

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d-dimensional spherical harmonics

- Effective radial Schrödinger equation for $\chi_{n,l}(r)$

$$-\frac{1}{2}\frac{d^2\chi_{n,l}(r)}{dr^2}+\left[V(r)+\frac{(l+\frac{d-3}{2})(l+\frac{d-1}{2})}{2\,r^2}\right]\chi_{n,l}(r)=\epsilon_{n,l}\,\chi_{n,l}(r)\quad,\quad r\geq 0$$

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Back to the CDF of $r_{\max}$ using spherical coordinates

$$Q_d(M,N) = \Pr(r_{\max} \le M) = \Pr[r_1 \le M, r_2 \le M, \ldots, r_N \le M]$$

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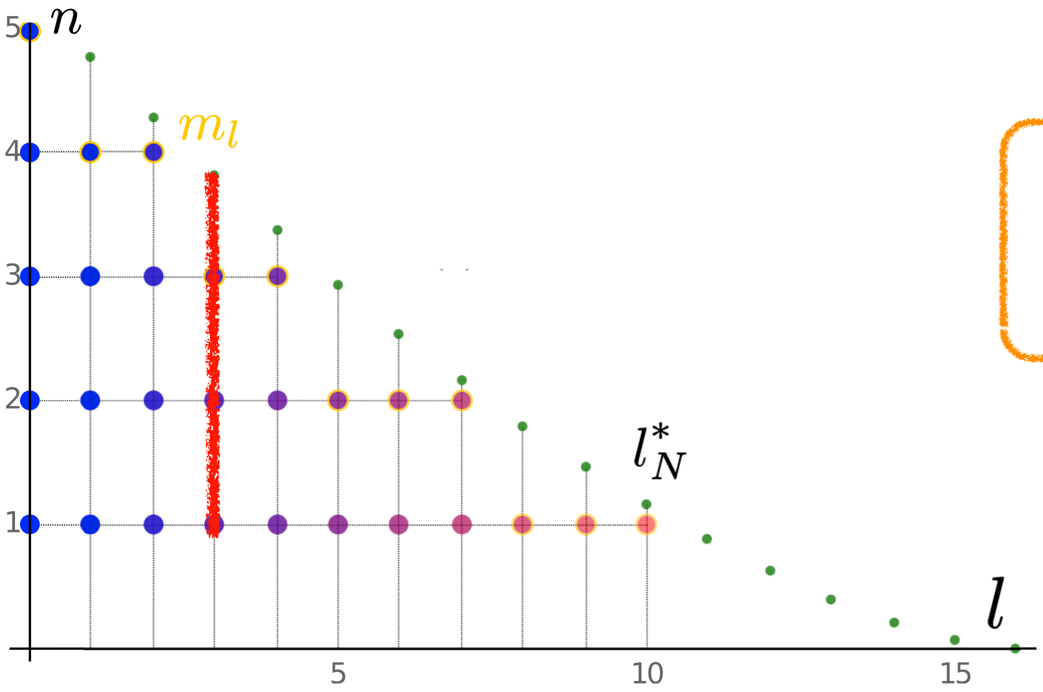
the determinant has a block structure

CDF of $r_{\max}$ using spherical coordinates

- Taking into account the degeneracy $g_d(l)$



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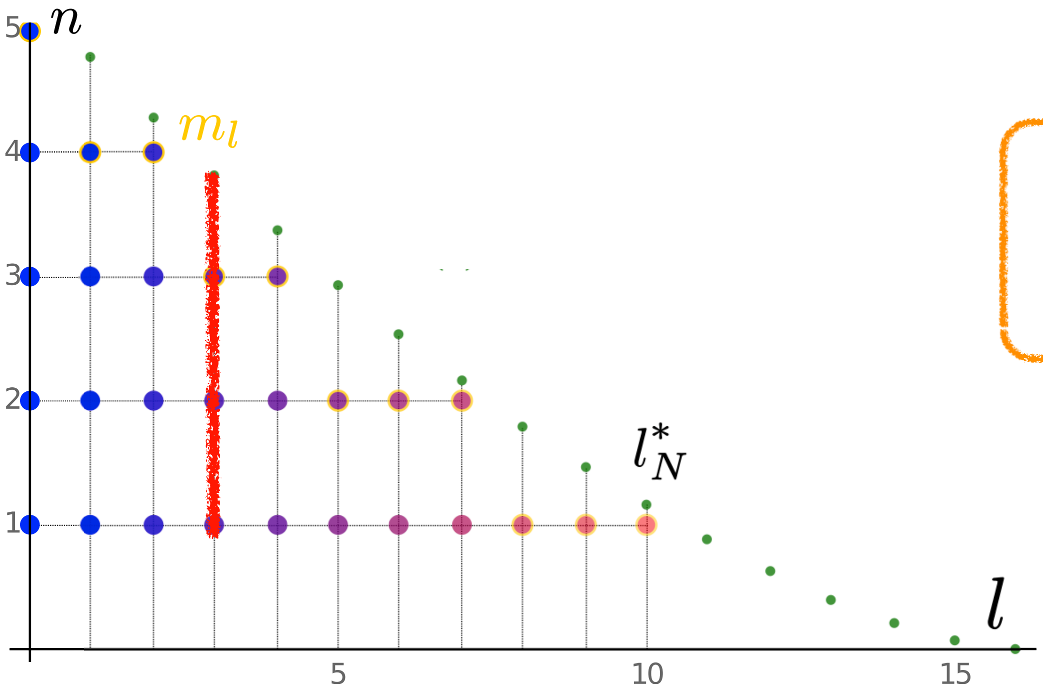

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⟹ different l-sectors decouple

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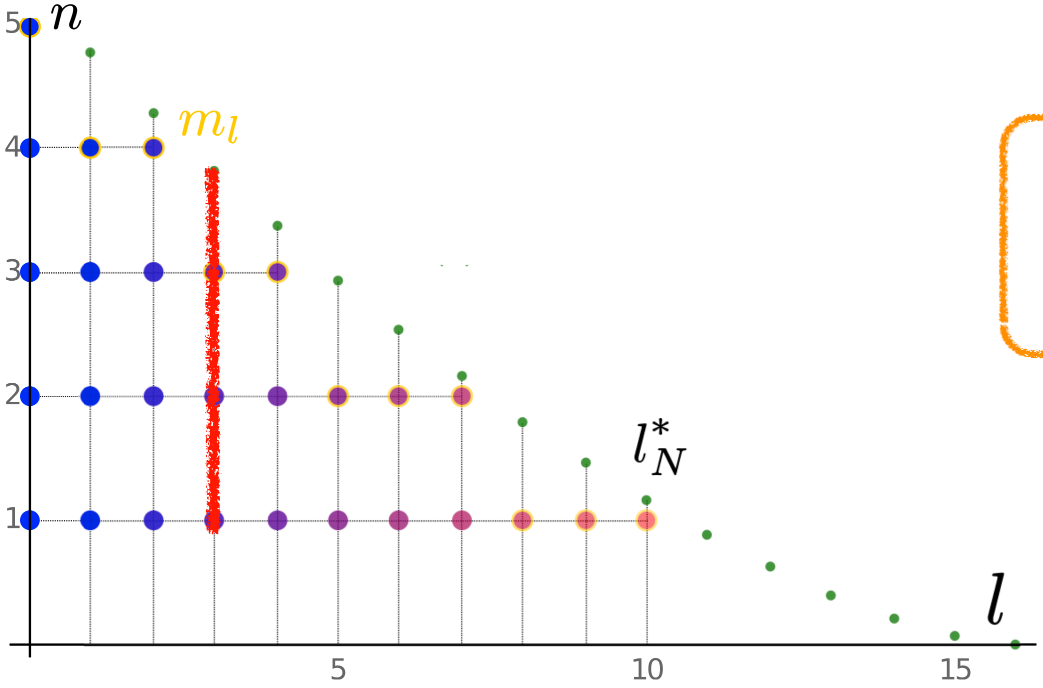

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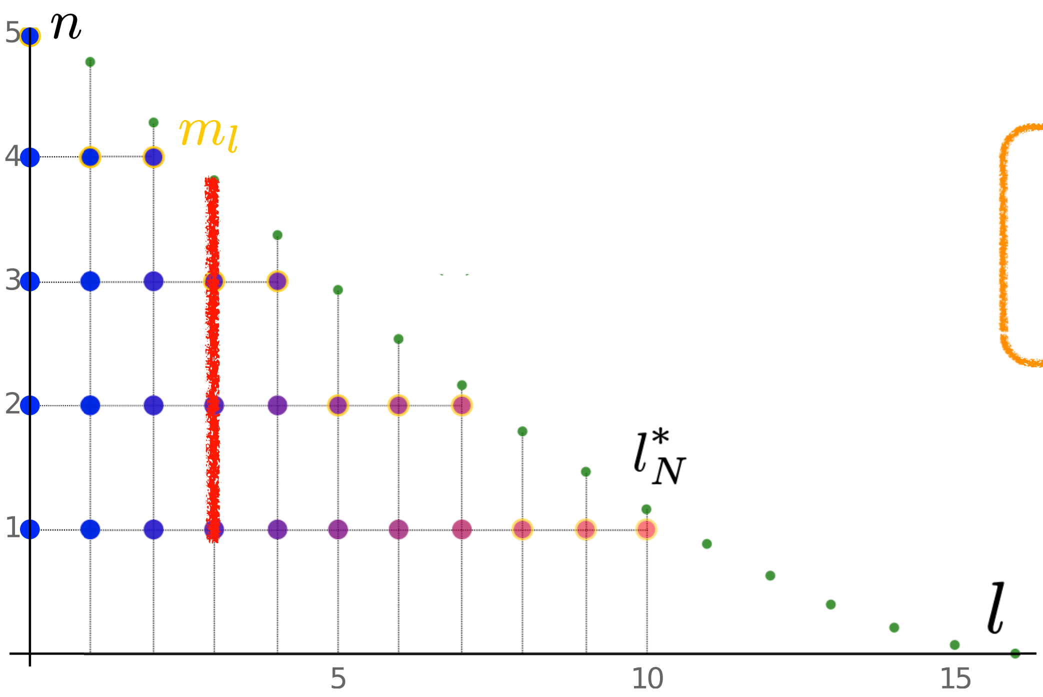

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CDF of the position of the rightmost fermion (among m_l) in an effective hard box 1d potential

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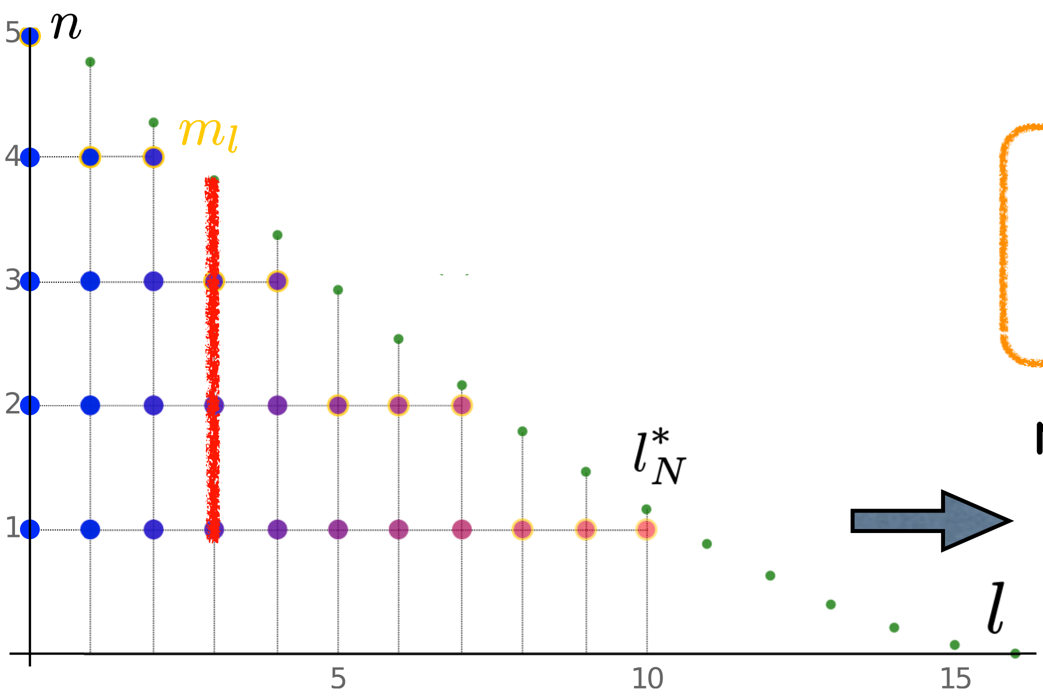

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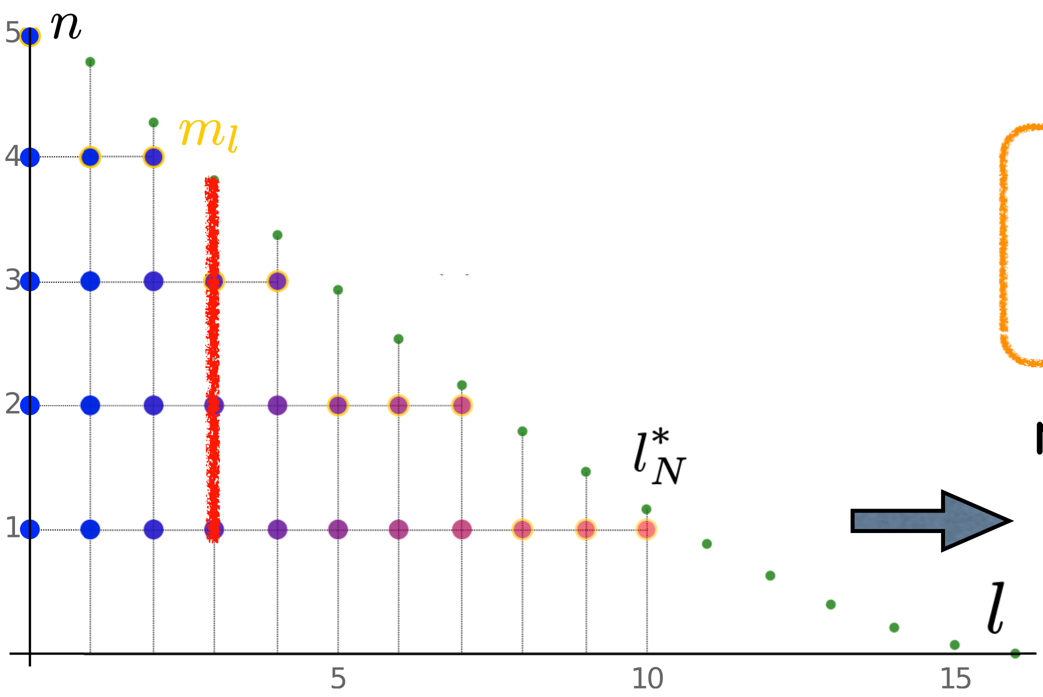
cf B. Lacroix-A-Chez-Toine 's talk



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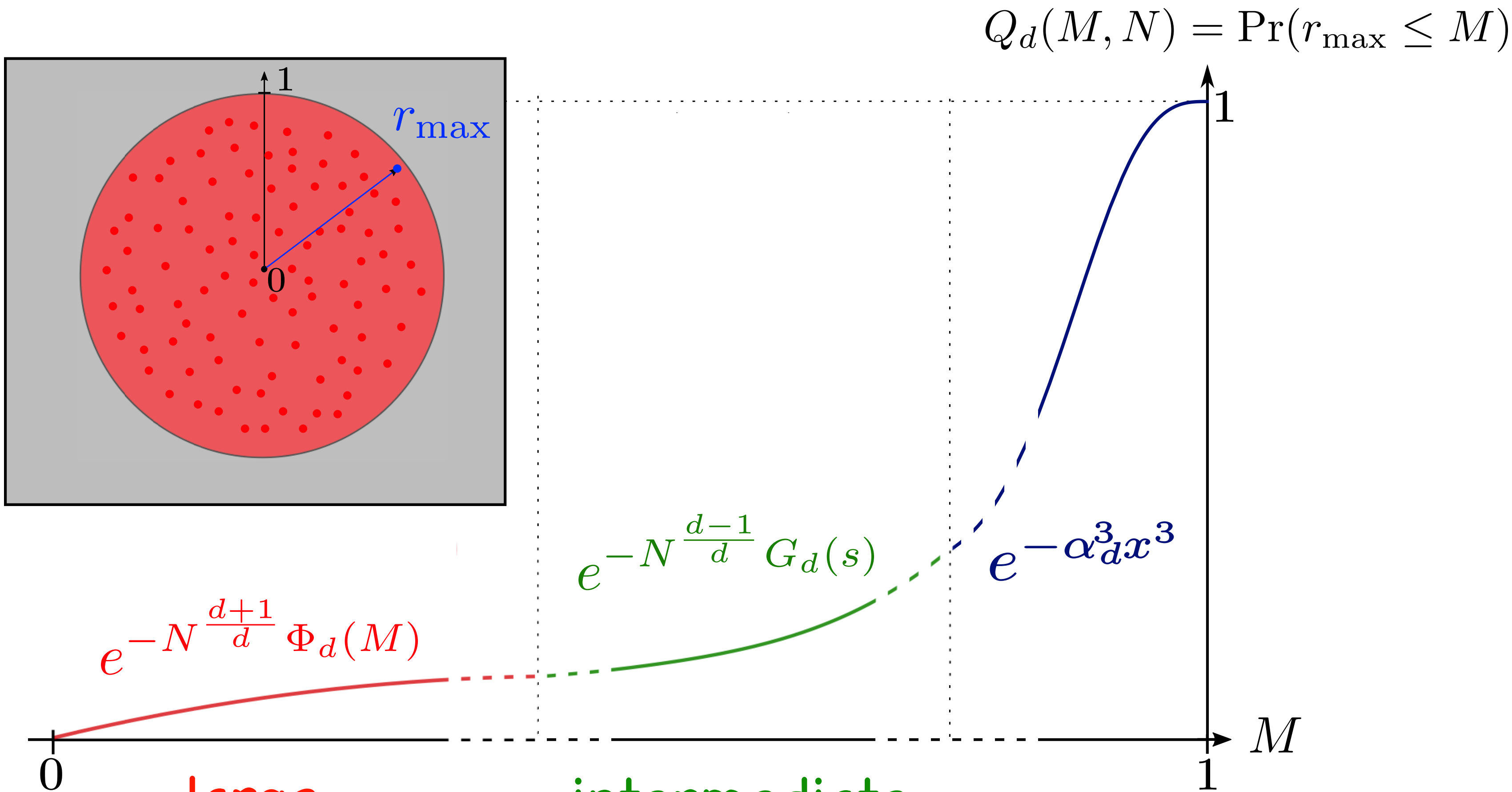
Radial distance of the farthest fermion in d>1

A smooth matching between the three regimes



large deviations

$(1-M) = O(1)$

intermediate deviations

$(1-M) = s\,N^{-\frac{1}{d}}$

typical

$(1-M) = x\,N^{-\frac{d+2}{3d}}$

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B. Lacroix-A-Chez-Toine, P. Le Doussal, S. N. Majumdar, G. S. '17

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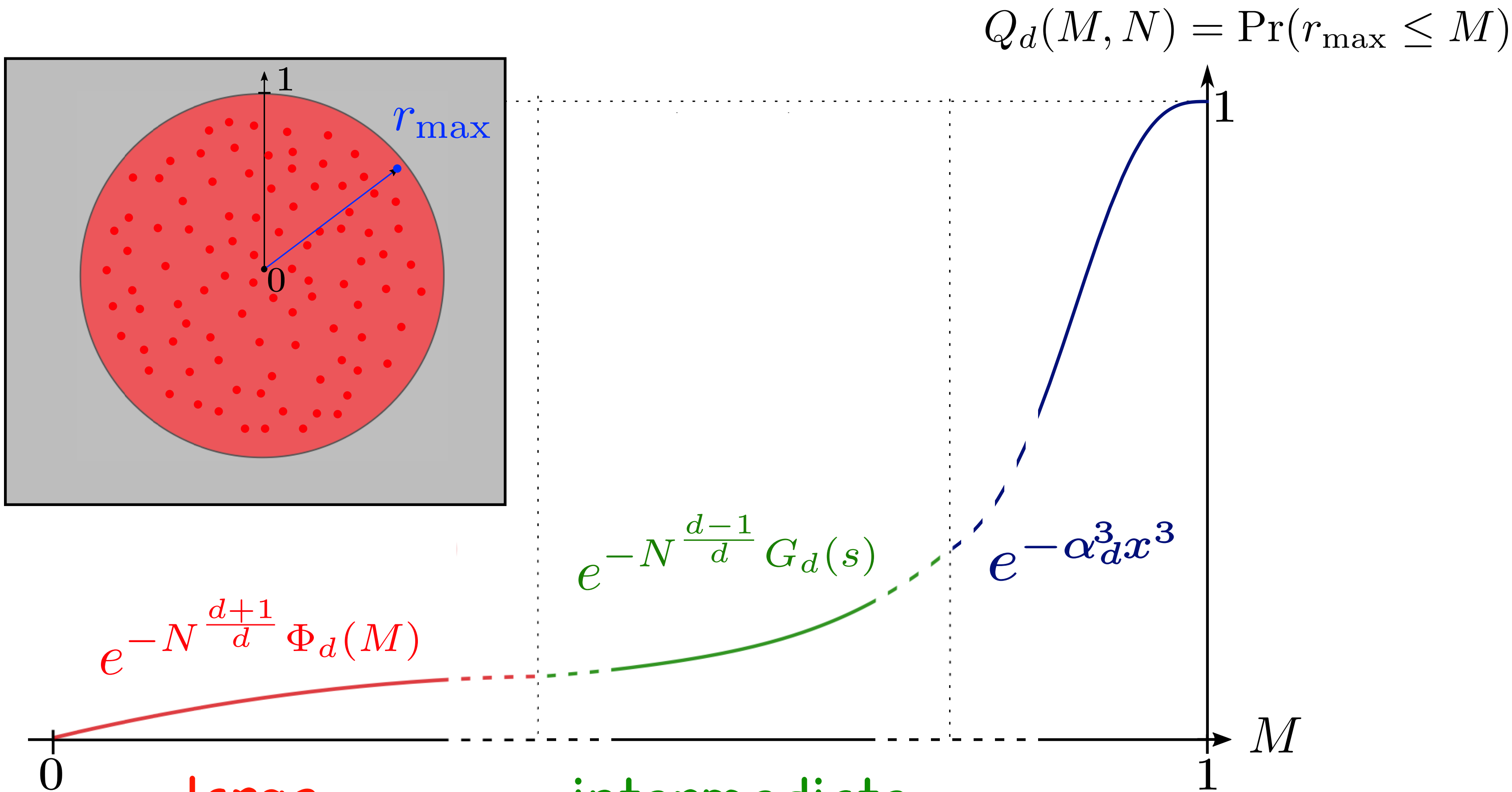

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- Can one observe these properties in cold atoms experiments ?

Free fermions in a d-dimensional harmonic trap (T=0): limiting correlation kernels

$$K_N(\mathbf{x},\mathbf{y}) = \sum_{\mathbf{k}} \theta(E_F - \epsilon_{\mathbf{k}})\psi_{\mathbf{k}}(\mathbf{x})\psi_{\mathbf{k}}(\mathbf{y})$$

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$$K_N(\mathbf{x},\mathbf{y}) \approx \frac{1}{w_N^d}\mathcal{K}_{\text{edge}}\left(\frac{\mathbf{x}-\mathbf{r}_{\text{edge}}}{w_N}, \frac{\mathbf{y}-\mathbf{r}_{\text{edge}}}{w_N}\right)$$

with $$\boxed{\mathcal{K}_{\text{edge}}(\mathbf{a},\mathbf{b}) = \int \frac{d^d q}{(2\pi)^d} e^{-i\mathbf{q}\cdot(\mathbf{a}-\mathbf{b})} Ai_1\left(2^{\frac{2}{3}}q^2 + \frac{a_n+b_n}{2^{1/3}}\right)}$$

$a_n = \mathbf{a}\cdot\mathbf{r}_{\text{edge}}/r_{\text{edge}}$ and $b_n = \mathbf{b}\cdot\mathbf{r}_{\text{edge}}/r_{\text{edge}}$

$$Ai_1(z) = \int_z^\infty Ai(u)\,du$$

Outline

- Free fermions in d=1 and T=0 and Random Matrix Theory (RMT)

- Free fermions in d=1 and T>0 and KPZ equation: main results

- Sketch of the derivation of our results

- Extension to higher dimensions, d>1

- Conclusion

Average density of free fermions at T > 0

$$P_{\text{joint}}(x_1, \cdots x_N) = \frac{1}{N! Z_N(\beta)} \sum_{k_1 < \cdots < k_N} \left[\det_{1 \le i,j \le N} (\varphi_{k_i}(x_j)) \right]^2 e^{-\beta(\epsilon_{k_1} + \cdots + \epsilon_{k_N})}$$

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$$\rho_N(x,T) = \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_N \, P_{\text{joint}}(x, x_2, \cdots, x_N)$$

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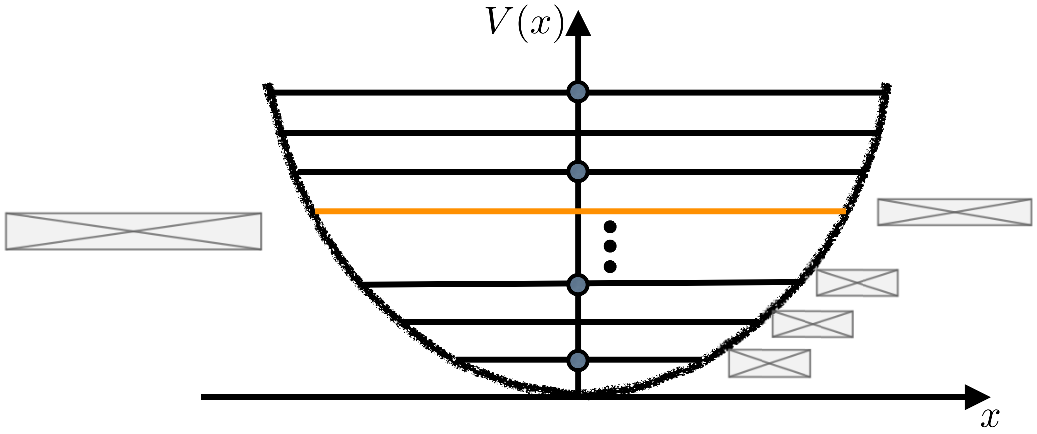
introduce the occupation numbers



$$m_k = \begin{cases} 0 \, , & \text{if state } k \text{ is empty} \\ 1 \, , & \text{if state } k \text{ is occupied} \end{cases}$$

Average density of free fermions at T > 0

$$P_{\rm joint}(x_1,\cdots x_N) = \frac{1}{N! Z_N(\beta)} \sum_{k_1<\cdots<k_N} \left[\det_{1\le i,j\le N}(\varphi_{k_i}(x_j))\right]^2 e^{-\beta(\epsilon_{k_1}+\cdots+\epsilon_{k_N})}$$

- Exact expression for the av. density $\rho_N(x,T) = \frac{1}{N}\sum_{i=1}^{N}\langle\delta(x-x_i)\rangle$

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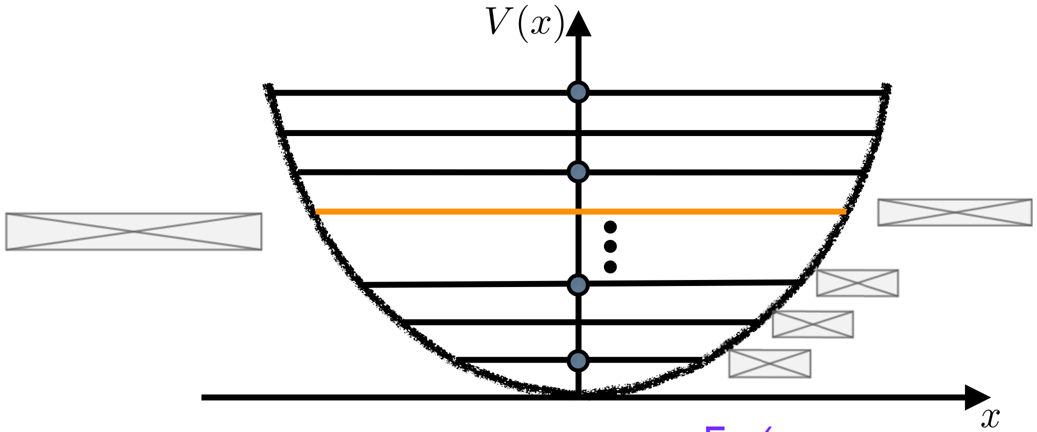

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$$\rho_N(x) = \frac{1}{Z_N(\beta)}\frac{1}{N}\sum_{\{m_k\}}\left[\left(\sum_{k\ge 0} m_k(\varphi_k(x))^2\right) e^{-\beta\sum_{k\ge0} m_k\epsilon_k}\delta\left(\sum_{k\ge0} m_k, N\right)\right]$$

Average density of free fermions at T > 0

$$\rho_N(x) = \frac{\mathcal{N}_N(x)}{N Z_N(\beta)}$$ with $$\mathcal{N}_N(x) = \sum_{\{m_k\}} \left[\left(\sum_{k\geq 0} m_k (\varphi_k(x))^2 \right) e^{-\beta \sum_{k\geq 0} m_k \epsilon_k} \delta\left(\sum_{k\geq 0} m_k, N \right) \right]$$

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- Generating function: grand-canonical ensemble, with $z = e^{\beta\mu}$

$$\sum_{N\geq 0} z^N \mathcal{N}_N(x) = \sum_{\{m_k\}} \sum_{k\geq 0} m_k (\varphi_k(x))^2 e^{-\beta \sum_{k\geq 0} m_k \epsilon_k} z^{\sum_{k\geq 0} m_k}$$

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$$= \sum_{k\geq 0} (\varphi_k(x))^2 z\, e^{-\beta\epsilon_k} \prod_{j\neq k} \left[\sum_{m_j=0}^{1} e^{-\beta m_j \epsilon_j} z^{m_j} \right]$$

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$$\begin{aligned}
\sum_{N\geq 0} z^N \mathcal{N}_N(x) &= \sum_{\{m_k\}} \sum_{k\geq 0} m_k (\varphi_k(x))^2 e^{-\beta \sum_{k\geq 0} m_k \epsilon_k} z^{\sum_{k\geq 0} m_k} \\
&= \sum_{k\geq 0} (\varphi_k(x))^2 z\, e^{-\beta\epsilon_k} \prod_{j\neq k} \left[\sum_{m_j=0}^{1} e^{-\beta m_j \epsilon_j} z^{m_j} \right] \\
&= \prod_{j=0}^{\infty} [1 + z\, e^{-\beta\epsilon_j}] \sum_{k\geq 0} (\varphi_k(x))^2 \frac{z\, e^{-\beta\epsilon_k}}{1 + z\, e^{-\beta\epsilon_k}}
\end{aligned}$$

Average density of free fermions at T > 0

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similarly $\displaystyle\sum_{N\geq 0} z^N Z_N(\beta) = \prod_{j=0}^{\infty} (1 + z\, e^{-\beta\epsilon_j})$ grand-canonical partition function

Average density of free fermions at T > 0

- An exact formula (using Cauchy formula)

$$\rho_N(x) = \frac{1}{N} \frac{\oint \frac{dz}{2i\pi} z^{-(N+1)} \prod_{j=0}^{\infty}(1+z\, e^{-\beta\epsilon_j}) \sum_{k\geq 0}(\varphi_k(x))^2 \frac{z\, e^{-\beta\epsilon_k}}{1+z\, e^{-\beta\epsilon_k}}}{\oint \frac{dz}{2i\pi} z^{-(N+1)} \prod_{j=0}^{\infty}(1+z\, e^{-\beta\epsilon_j})}$$

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$$\rho_N(x) \underset{N\to\infty}{\approx} \frac{1}{N} \sum_{k\geq 0} (\varphi_k(x))^2 \frac{z^* e^{-\beta\epsilon_k}}{1+z^* e^{-\beta\epsilon_k}}$$

via saddle-point calculation

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Setting $z^* = e^{\beta\mu}$ one has $$\frac{z^* e^{-\beta\epsilon_k}}{1+z^* e^{-\beta\epsilon_k}} = \frac{1}{e^{\beta(\epsilon_k-\mu)}+1} = \langle m_k \rangle$$

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Fermi factor

Correlation kernel for free fermions at T > 0

- Final result for the density for large N

$$\rho_N(x) \approx \frac{1}{N} \sum_{k \geq 0} (\varphi_k(x))^2 \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}$$

Correlation kernel for free fermions at T > 0

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- ⊠-point correlation functions for large N (by similar computations)

$$R_n(x_1, \cdots, x_n) \approx \det_{1 \leq i,j \leq n} K_N(x_i, x_j)$$

where the correlation kernel is given by

$$K_N(x, x') = \sum_{k=0}^{\infty} \frac{\varphi_k(x)\varphi_k(x')}{e^{\beta(\epsilon_k - \mu)} + 1} \qquad \text{and} \qquad N = \sum_{k=0}^{\infty} \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}$$

Average density of free fermions at T > 0

$$\rho_N(x,T) = \frac{1}{N}\sum_{i=1}^{N}\langle\delta(x-x_i)\rangle$$

- Two natural dimensionless variables

$$y = \frac{E_F}{T} = \frac{N\hbar\,\omega}{T} \qquad \text{and} \qquad z = x\sqrt{\frac{m\omega^2}{2\,T}}$$

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$$\rho_N(x,T) \sim \frac{\alpha}{\sqrt{N}} R\left(\frac{N\hbar\omega}{T} = y, x\sqrt{\frac{m\,\omega^2}{2T}} = z\right),$$

$$R(y,z) = -\frac{1}{\sqrt{2\pi\, y}}\mathrm{Li}_{1/2}\left(-\left(e^y-1\right)\,e^{-z^2}\right) \qquad \mathrm{Li}_n(x) = \sum_{k=1}^{\infty}\frac{x^k}{k^n}$$

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See also Local Density (or Thomas-Fermi) Approx. in the literature on fermions