University of Antwerp

The quantum canonical ensemble: a projection operator treatment

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Outline

- Motivation
- Free bosons and fermions in the canonical ensemble . . . a long standing problem
- A projection operator for the dirty work
- Exact results
- Two-dimensional electron gas
- Conclusion and outlook

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Motivation

Why should the canonical ensemble (CE) bother us?

Seriously?

*Because the **grand-canonical ensemble (GCE)** has become an "addictive comfort zone" to condensed matter theorists.*

- Sometimes, the **exact** number of particles N (CE), rather than the **average** number of particles $\langle \hat{N} \rangle$ (GCE), can be considered fixed: isolated (super)conductors, single-electron transistors, etc.
- For small $\langle \hat{N} \rangle$ (nanostructures), the GCE fluctuations of $\langle \hat{N} \rangle$ become too large compared to $\langle \hat{N} \rangle$.
- A critical review of approximation schemes that rely on the absence of particle number conservation – and hence on the GCE – would be highly recommended.

Motivation

Why should non-interacting particles bother us?

Confronting answer:
because our brains fail to cope with interacting particles.

Comforting answer:
because lots of approximation schemes still rely on non-interacting particle models:

- perturbation theory with un unperturbed Hamiltonian describing free particles,
- variational techniques, approximate canonical transformations, Hubbard – Stratonovich transforms, BCS theory, partial diagonalizations, Hartree-like Poisson – Schrödinger solvers . . .

Non-interacting systems are everything BUT trivial!

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Free bosons and fermions in the CE . . .

- **Canonical partition function for N identical particles**

$$Z_N = \mathrm{Tr}\left(\exp(-\beta \hat{\mathrm{H}}_N)\right), \quad \beta = 1/k_\mathrm{B}T$$

  – Calculating Z_N involves the diagonalization of the N-particle Hamiltonian $\hat{\mathrm{H}}_N$, yielding

$$Z_N = \sum_j \exp\left(-\beta E_{jN}\right), \quad \{E_{jN}\} = N\text{-particle energy eigenvalues}$$

  – Non-interacting (spinless) particles:

$$E_{jN} = \sum_k n_k \epsilon_k, \quad \epsilon_k = \text{single-particle energy eigenvalues,}$$

$$n_k = 0, 1, 2, 3, \ldots \text{ (bosons)} \qquad \text{or} \qquad n_k = 0, 1 \text{ (fermions).}$$

but ALWAYS

$$\boxed{\sum_k n_k = N}$$

Free bosons and fermions in the CE . . .

- **Canonical ensemble (CE) versus grand-canonical ensemble (GCE)**

<table>
<tr><th>CE</th><th>GCE</th></tr>
<tr><td>N fixed, $\langle \hat{N}^2 \rangle - N^2 = 0$</td><td>$\langle \hat{N} \rangle$ fixed, $\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 \neq 0$</td></tr>
<tr><td>Implicit chemical potential μ_N
but limited summation
$$Z_N = \sum_{\underbrace{n_1, n_2, \ldots}_{n_1+n_2+\ldots=N}} \exp(-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \ldots))$$
$$\neq \prod_k \left(\sum_{n_k} \exp(-\beta n_k \epsilon_k) \right)$$</td><td>Explicit chemical potential μ
but unlimited summation
$$Q(\mu) = \sum_{n_1, n_2, \ldots} \exp(-\beta(n_1(\epsilon_1 - \mu)) \times \exp(-\beta(n_2(\epsilon_2 - \mu)) \times \ldots$$
$$= \prod_k \left(\sum_{n_k} \exp(-\beta n_k(\epsilon_k - \mu)) \right)$$</td></tr>
</table>

Free bosons and fermions in the CE . . .

- **Feynman's warning from the past**

A state of the system is described by the set of numbers n_a, which can take on any set of values allowed both by the statistics and by the condition $\sum_a n_a = N$.

$$Q = \sum_{n_1, n_2, \ldots} \exp\left(-\beta \sum_a n_a \varepsilon_a\right). \tag{1.42}$$

If there were no restriction on the number of particles, we could write

$$Q = \prod_a \left(\sum_{n_a} e^{-\beta n_a \varepsilon_a}\right), \tag{1.43}$$

and we would have in the Bose-Einstein case

R. P. Feynman, "*Statistical Mechanics*", W. A. Benjamin, Inc., 1972, page 26.

Free bosons and fermions in the CE . . .

- **Some "canonical" work at TQC in the recent past**
  - F. Brosens, J. T. Devreese, and L. F. Lemmens, *"Canonical Bose-Einstein condensation in a parabolic well"*, Solid-St. Commun. **100**, 123 – 127 (1996).
  - J. Tempere and J. T. Devreese, *"Canonical Bose-Einstein condensation of interacting bosons in two dimensions"*, Solid-St. Commun. **101**, 657 – 659 (1997).
  - L. Lemmens, F. Brosens, and J. Devreese, *"Statistical mechanics and path integrals for a finite number of bosons"*, Solid-St. Commun. **109**, 615 – 620 (1999).

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A projection operator . . .

- **Operators in Fock space**
  - *The particle number operator* $\hat{\mathrm{N}}$ *and the many-particle Hamiltonian* $\hat{\mathrm{H}}$ *are beneficially represented by their second-quantized forms.*
  - ***Advantage:***
    second quantization naturally and automatically encoding particle permutation symmetry,

    $\updownarrow$

    first quantization “manually” bringing up Slater determinants and permanents.
  - ***Drawback:***
    Fock space ignores (fixed) particle numbers.
  - ***Escape route:***
    invoking a projection onto the subspace of N-particle states.

A projection operator . . .

- **Fiddling around with the restricted summation**

$$Z_N = \underbrace{\sum_{n_1, n_2, \ldots}}_{n_1+n_2+\ldots=N} \exp(-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \ldots))$$

$$= \sum_{n_1, n_2, \ldots} \exp(-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \ldots))\, \boldsymbol{\delta_{n_1+n_2+\ldots,\, N}}$$

$$= \sum_{n_1, n_2, \ldots} \exp(-\beta(n_1\epsilon_1 + n_2\epsilon_2 + \ldots)) \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta\, \exp(\mathrm{i}(n_1 + n_2 + \ldots - N)\theta)$$

$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta\, \exp(-\mathrm{i}N\theta) \sum_{n_1, n_2, \ldots} \exp((\mathrm{i}\theta - \beta\epsilon_1)n_1)\, \exp((\mathrm{i}\theta - \beta\epsilon_2)n_2) \times \ldots$$

$$= \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta\, \exp(-\mathrm{i}N\theta) \prod_k \sum_{n_k} \exp((\mathrm{i}\theta - \beta\epsilon_k)n_k)$$

A projection operator . . .

- **Projection operator**

  Same story, but now the posh way of telling . . .

$$\hat{\mathsf{P}}_N = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}\theta \, \exp\left(\mathrm{i}(\hat{\mathsf{N}} - N)\,\theta\right)$$

$$\Downarrow$$

$\hat{\mathsf{N}} \left(\hat{\mathsf{P}}_N \, |\psi\rangle\right) = N \left(\hat{\mathsf{P}}_N \, |\psi\rangle\right)$ for any state $|\psi\rangle$ in Fock space.

$$\Downarrow$$

  – $\hat{\mathsf{P}}_N$ projects any state onto the N-particle sub-space.
  – The N-particle Hamiltonian is the projected "Fock Hamiltonian": $\hat{\mathsf{H}}_N = \hat{\mathsf{P}}_N \hat{\mathsf{H}} \, \hat{\mathsf{P}}_N$.

A projection operator ...

- **Recasting the CE partition function**
  - *Under the (reasonable) assumption* $[\hat{\mathsf{H}}, \hat{\mathsf{N}}] = 0$ *it follows that*

$$\exp(-\beta\,\hat{\mathsf{H}}_N) = \exp(-\beta\,\hat{\mathsf{P}}_N \hat{\mathsf{H}}\,\hat{\mathsf{P}}_N) = \hat{\mathsf{P}}_N \exp(-\beta\,\hat{\mathsf{H}})\,\hat{\mathsf{P}}_N$$

$$\Downarrow$$

$$Z_N(\beta) = \mathrm{Tr}\left(\hat{\mathsf{P}}_N \exp(-\beta\,\hat{\mathsf{H}})\right)$$

  - ***Generating function***

$$G(\beta,\theta) = \mathrm{Tr}\left(\exp\left(\mathrm{i}\hat{\mathsf{N}}\theta\right)\exp(-\beta\,\hat{\mathsf{H}})\right)$$

  - *Partition function =* N*-th Fourier coefficient of* $G(\beta,\theta)$

$$Z_N(\beta) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\theta\,\exp(-\mathrm{i}N\theta)\,G(\beta,\theta),$$

A projection operator . . .

- **Non-interacting particles (1/3)**

  – *Particle statistics tag ξ*

$\xi = 1$	bosons
$\xi = -1$	fermions

  – *Creation / destruction operators – (anti)commutation relations*

$$c_k c_{k'} - \xi c_{k'} c_k = c_k^\dagger c_{k'}^\dagger - \xi c_{k'}^\dagger c_k^\dagger = 0, \quad c_k c_{k'}^\dagger - \xi c_{k'}^\dagger c_k = \delta_{k,k'}$$

  – *Other operators* $\hat{\mathrm{H}} = \sum_k \epsilon_k c_k^\dagger c_k, \quad \hat{\mathrm{N}} = \sum_k c_k^\dagger c_k$

  – ***Factorizing the generating function, freed from summation restrictions***

$$G(\beta,\theta) = \prod_k \mathrm{Tr} \exp\left((\mathrm{i}\theta - \beta\epsilon_k)\, c_k^\dagger c_k\right)$$
$$= \prod_k \sum_{n_k} \exp\left((\mathrm{i}\theta - \beta\epsilon_k)\, n_k\right)$$

A projection operator . . .

- **Non-interacting particles (2/3)**
  - *Generating function as a product over all single-particle modes* k

$$G(\beta, \theta) = \left[\prod_k \left(1 - \xi \exp\left(\mathrm{i}\theta - \beta\epsilon_k\right)\right) \right]^{-\xi}$$

  - *Fourier representation of* $Z_N(\beta)$ *is equivalent with a complex contour integral*

$$Z_N(\beta) = \frac{1}{2\pi\mathrm{i}} \oint_\Gamma \frac{\mathrm{d}z}{z^{N+1}} \tilde{G}(\beta, z), \qquad \tilde{G}(\beta, z) \equiv \left[\prod_k \left(1 - \xi z \exp\left(-\beta\epsilon_k\right)\right) \right]^{-\xi}.$$

Γ is a closed contour encircling $z = 0$, $\tilde{G}(\beta, z)$ being analytic inside Γ, e.g. $|z| = 1$.

$\Downarrow$

An old recursion relation can be rederived in a few lines.

A projection operator . . .

- **Non-interacting particles (3/3)**
  - *Previously known recursion relation*

$$Z_0(\beta) = 1, \quad Z_1(\beta) = \sum_k \exp(-\beta\epsilon_k),$$

$$Z_N(\beta) = \frac{1}{N}\sum_{l=1}^{N} \xi^{l-1} Z_1(l\beta)\, Z_{N-l}(\beta) \quad \text{for } N \geqslant 1.$$

  - *Correlation functions*

    Projector approach + commutator algebra = generic expressions for 2-point and 4-point correlation functions, e.g.

$$\langle c_q^\dagger\, c_{q'}^\dagger\, c_{k'}\, c_k \rangle_\beta = \frac{1}{2\pi Z_N}\left(\xi\delta_{kq}\delta_{k'q'} + \delta_{kq'}\delta_{k'q}\right)\int_{-\pi}^{\pi} \mathrm{d}\theta\, \exp\left(-\mathrm{i}N\theta\right)$$
$$\times \frac{G(\beta,\theta)}{\left(\exp\left(\beta\epsilon_k - \mathrm{i}\theta\right) - \xi\right)\left(\exp\left(\beta\epsilon_{k'} - \mathrm{i}\theta\right) - \xi\right)}.$$

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Exact results

- **One-dimensional oscillators (1/3)**
  - *Harmonic potential :* $U(x) = \frac{1}{2} m\omega^2 x^2$
  - *Single-particle spectrum:* $\epsilon_k = \hbar\omega\left(k + \frac{1}{2}\right), \quad k = 0, 1, 2, 3, \ldots$
  - *Exact results derived from projection technique and two Euler identities*
  - ***Partition function***

$$Z_N(\beta) = \begin{cases} e^{-N\beta\hbar\omega/2} \prod_{k=1}^{N} \frac{1}{1 - e^{-\beta\hbar\omega k}} & \text{for bosons,} \\ e^{-N^2\beta\hbar\omega/2} \prod_{k=0}^{N} \left(1 - e^{-\beta\hbar\omega k}\right) & \text{for fermions.} \end{cases}$$

Exact results

- **One-dimensional oscillators (2/3)**

  – ***Helmholtz free energy***

$$F_N(\beta) = \frac{1}{\beta}\sum_{k=1}^{N} \ln\left(1 - e^{-\beta\hbar\omega k}\right) + \begin{cases} \frac{1}{2}N\hbar\omega & \text{for bosons,} \\ \frac{1}{2}N^2\hbar\omega & \text{for fermions.} \end{cases}$$

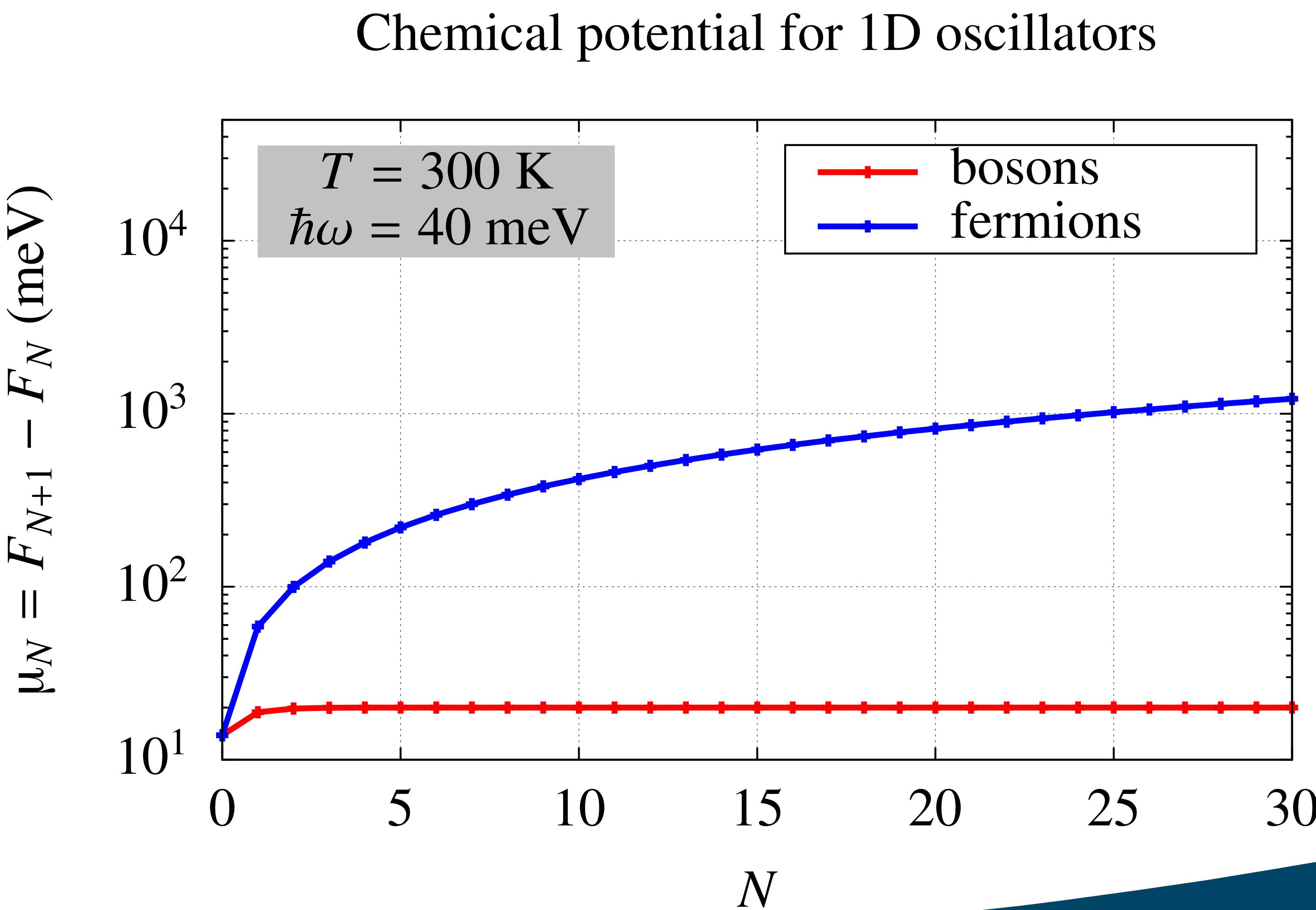
  – ***Chemical potential***

$$\mu_N(\beta) = F_{N+1}(\beta) - F_N(\beta)$$

$$= \frac{1}{\beta}\ln\left(1 - e^{-(N+1)\beta\hbar\omega}\right) + \begin{cases} \frac{1}{2}\hbar\omega & \text{for bosons,} \\ \left(N + \frac{1}{2}\right)\hbar\omega & \text{for fermions.} \end{cases}$$

Exact results

- **One-dimensional oscillators (3/3)**



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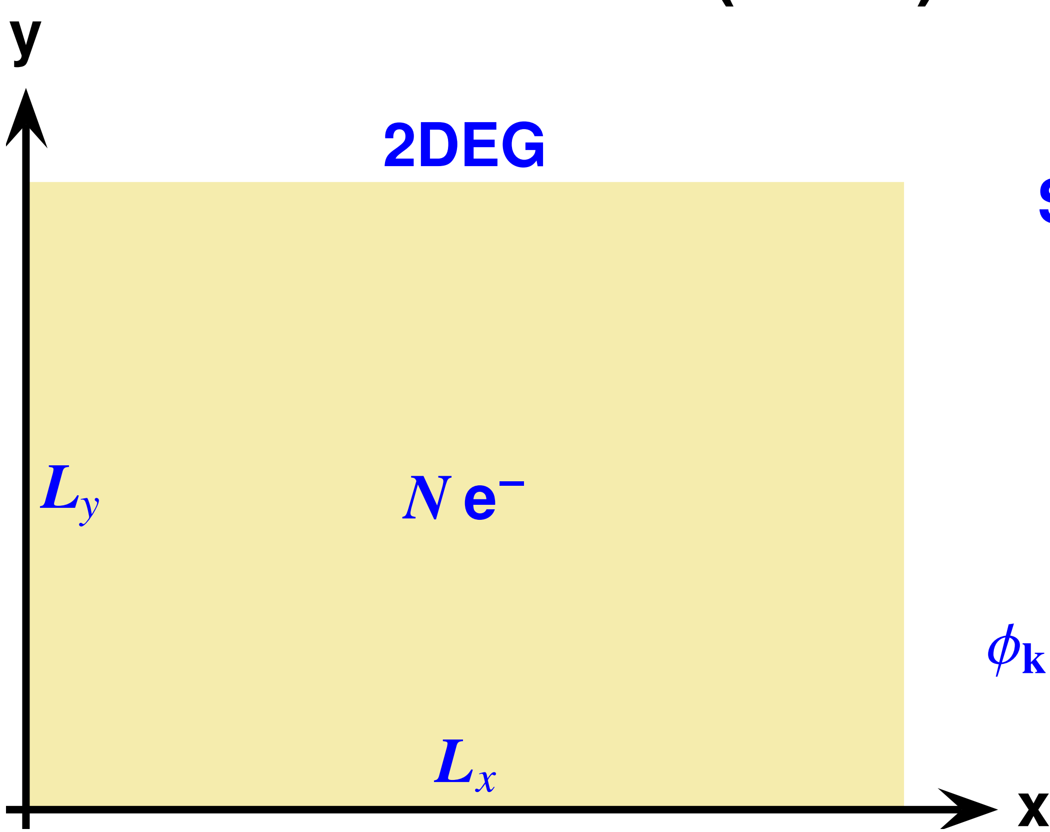
Two-dimensional electron gas

- **Free electrons on a (finite) sheet**



Single electron spectrum

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}$$

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{\exp(i\mathbf{k}\cdot\mathbf{r})}{\sqrt{L_x L_y}}$$

Periodic boundary conditions $\Rightarrow$ $\mathbf{k} = 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}\right), \ n_x, n_y = 0, \pm 1, \pm 2, \ldots$

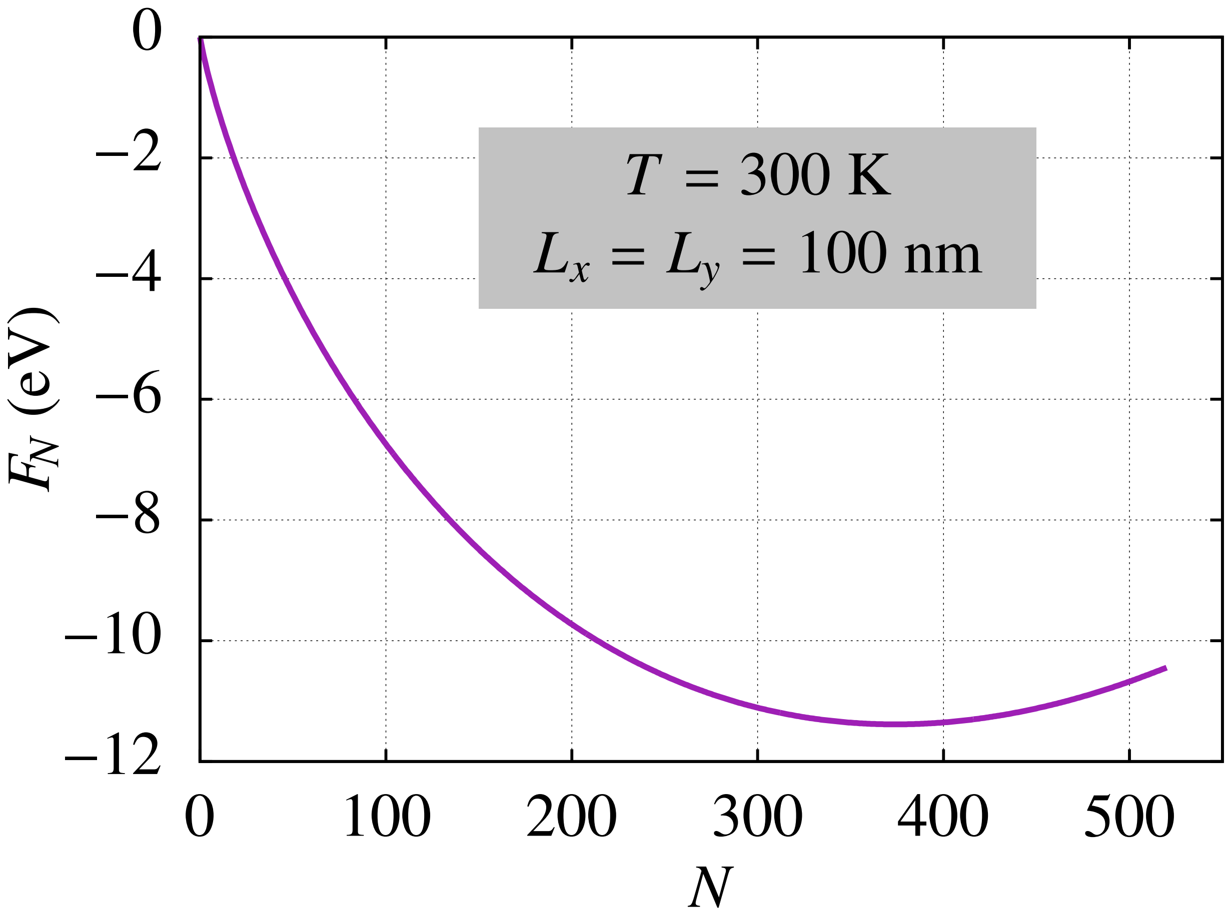
Areal concentration: $$\boxed{n_S = \frac{N}{L_x L_y}}$$

Two-dimensional electron gas

- **Helmholtz free energy**

$$F_N = -k_\mathrm{B} T \ln Z_N$$

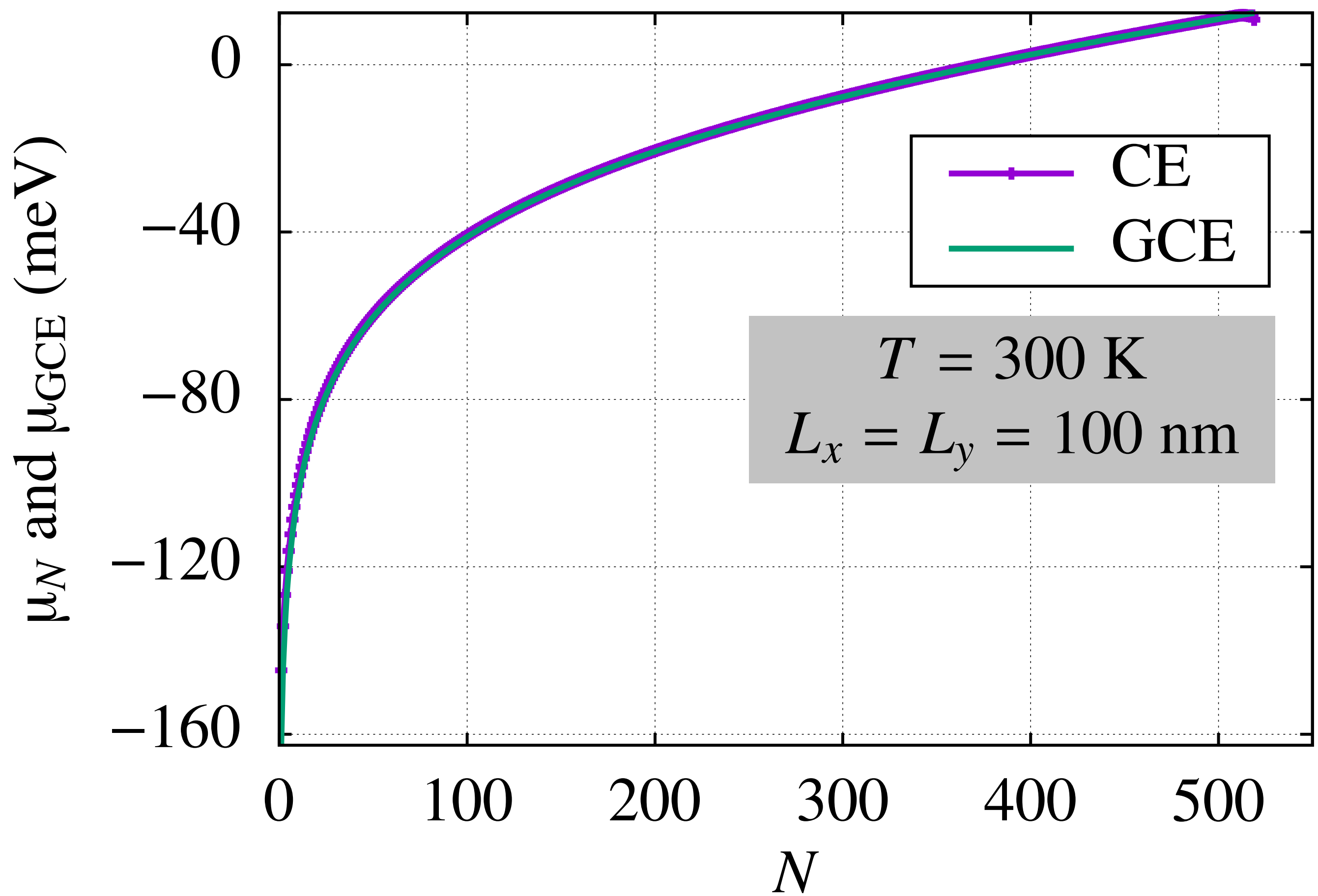
Numerical instability for $N > 520$.



Two-dimensional electron gas

- **Chemical potential (1/2)**

$$\mu_N = F_{N+1} - F_N$$



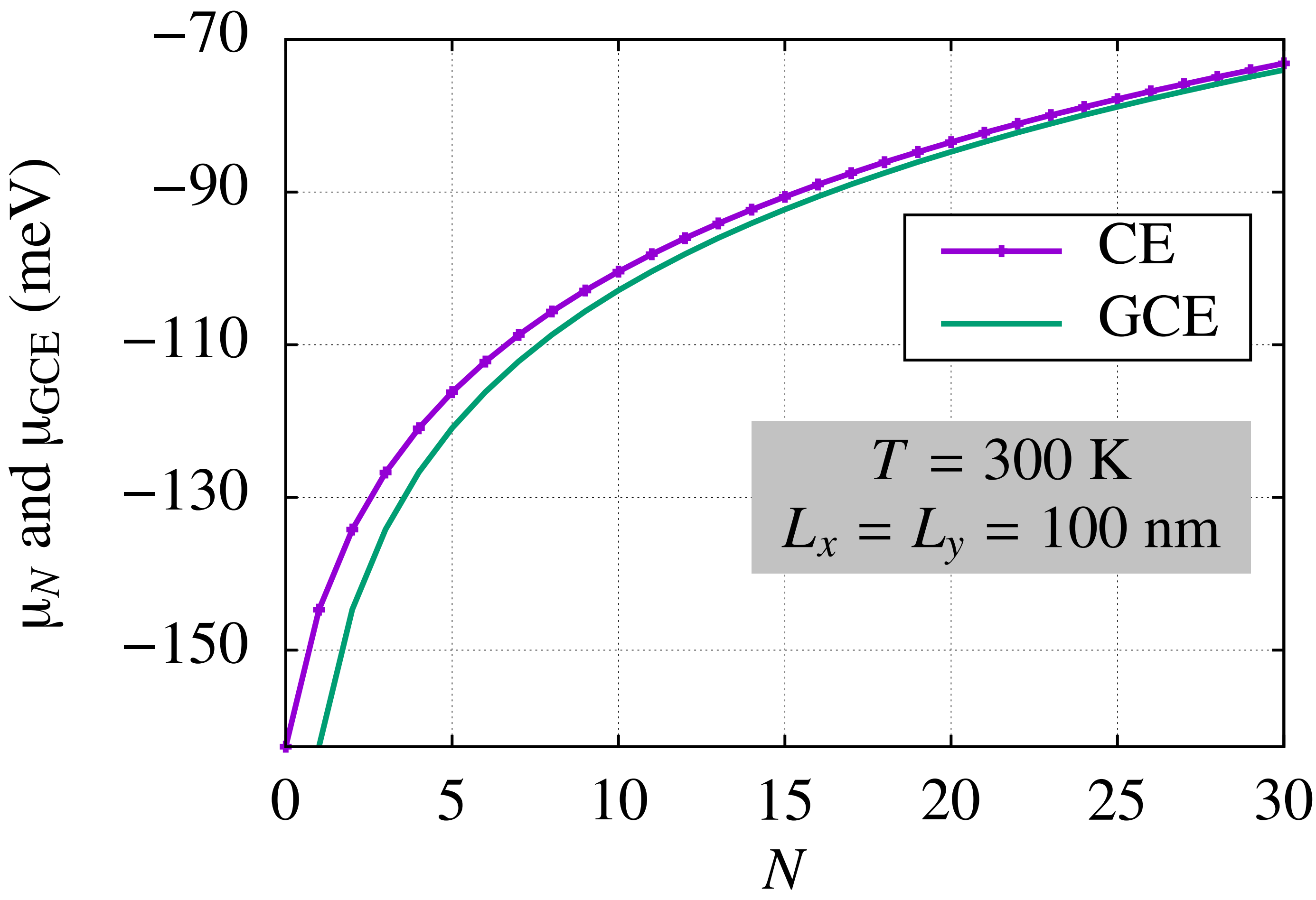
Two-dimensional electron gas

- **Chemical potential (2/2)**

$$\mu_N = F_{N+1} - F_N$$

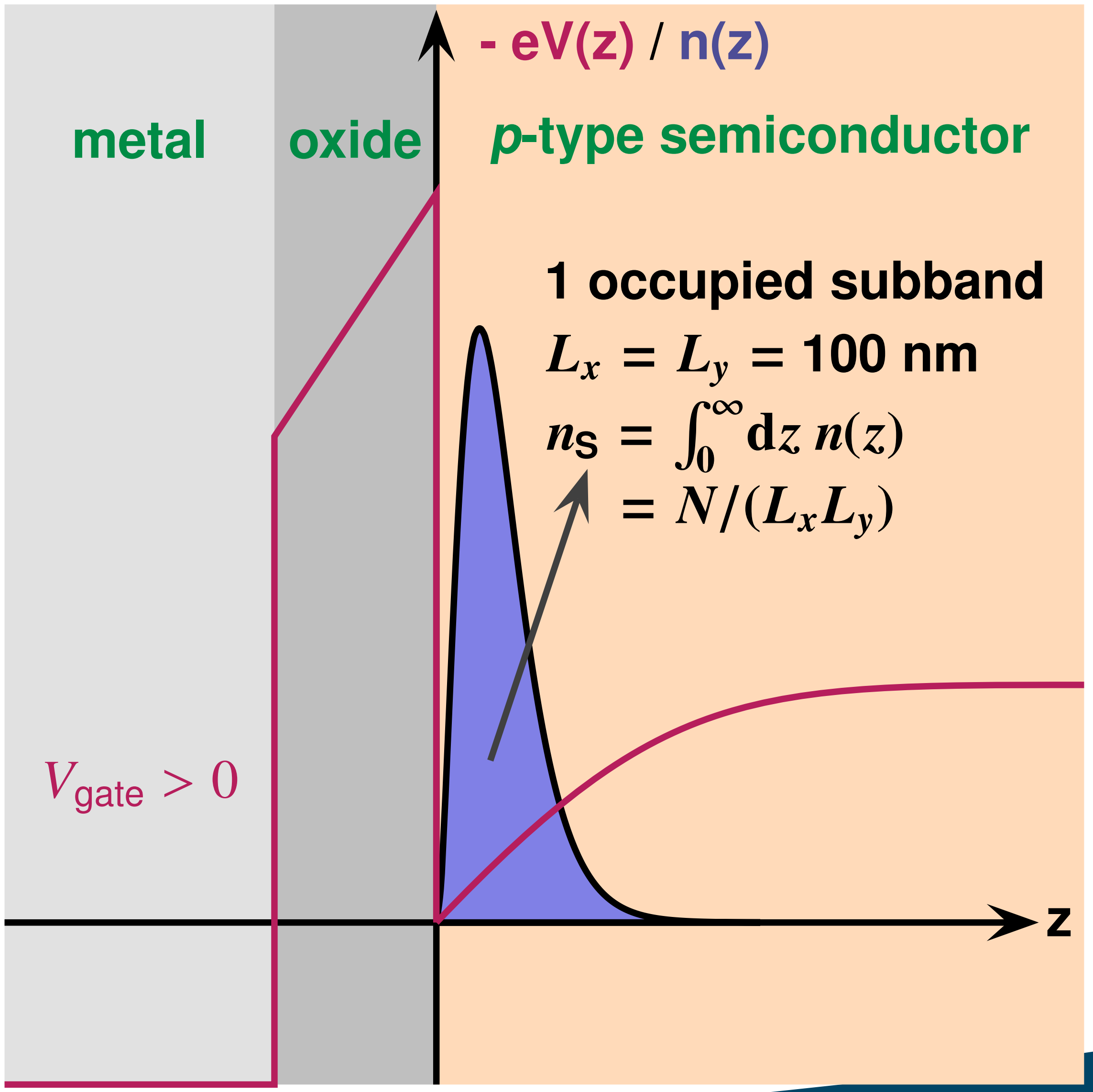
GCE unreliable for

$N < 20$



Two-dimensional electron gas

- **Application: *n*-channel MOS capacitor**



Free bosons and fermions in the CE . . .

- **Recent publications**
  - Wim Magnus, Lucien Lemmens, Fons Brosens, *“Quantum canonical ensemble: a projection operator approach”*, arXiv:1505.04923v2 [cond-mat.stat-mech] 22 Dec 2016.
  - Wim Magnus, Lucien Lemmens, Fons Brosens, *“Quantum canonical ensemble: A projection operator approach”*, Physica A **482**, 1 – 13 (2017).

Two-dimensional electron gas

- **Two caveats related to the GCE (1/2)**

  1. ***The GCE increases the numerical burden in device simulators***

     – Transcendental equation fixing the chemical potential μ for a given value of $\langle \hat{N} \rangle$ (or n_S for the MOSCAP):

$$\boxed{\langle \hat{N} \rangle = \sum_k \frac{1}{1 + \exp\left(\beta\left(\epsilon_k - \mu\right)\right)}} \Rightarrow \mu = \mu\left(\langle \hat{N} \rangle\right).$$

     – No analytical solution available in general, i.e. for an arbitrary potential and several occupied subbands.

     – The numerical solution is carried out in the **outer loops** of the Poisson-Schrödinger solver.

Two-dimensional electron gas

- **Two caveats related to the GCE (2/2)**

  2. ***The GCE is unreliable for small values of*** $\langle \hat{N} \rangle$.

     – The GCE variance $\sigma = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2$ is negligible only if $\langle \hat{N} \rangle \to \infty$.

     $\updownarrow$

     In an inversion layer covering a 100 nm x 100 nm active area n_S typically ranges between

     $$n_S = 10^{11}\text{cm}^{-2} \quad \Rightarrow \quad \langle \hat{N} \rangle = 10,$$

     $$n_S = 10^{12}\text{cm}^{-2} \quad \Rightarrow \quad \langle \hat{N} \rangle = 100,$$

     i.e. $\langle \hat{N} \rangle$ doesn't exactly take large values . . .

     – "Threshold voltage" models rely on the transition area between $n_S \approx 0$ and $n_S \approx 10^{11}$ cm^{-2}. i.e. the region where $\mu \to -\infty$.

     $\Rightarrow$ *unreliable estimates for the subthreshold slope in nanodevices.*

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Conclusion and outlook

+ The projector operator approach provides a tool to systematically investigate non-interacting fermions and bosons in the CE (incl. correlation functions).

+ All quantum systems containing a number of particles that can be considered fixed, can be accessed from the CE approach, e.g. nanostructures, quantum dots, quantum rings, SETs, superconducting, rings, BCS-like systems etc.

+ A by-product, μ_N needs not be extracted from a transcendental equation, as would be required for the GCE.

+ In practice, the calculation of Z_N and F_N is reduced to a numerical problem (angular integral, recursion relation).

– Attention needs to be paid to the numerical problems related to the evaluation of the angular or contour integrals, for “large” values of N.

Be grand. Be canonical.

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