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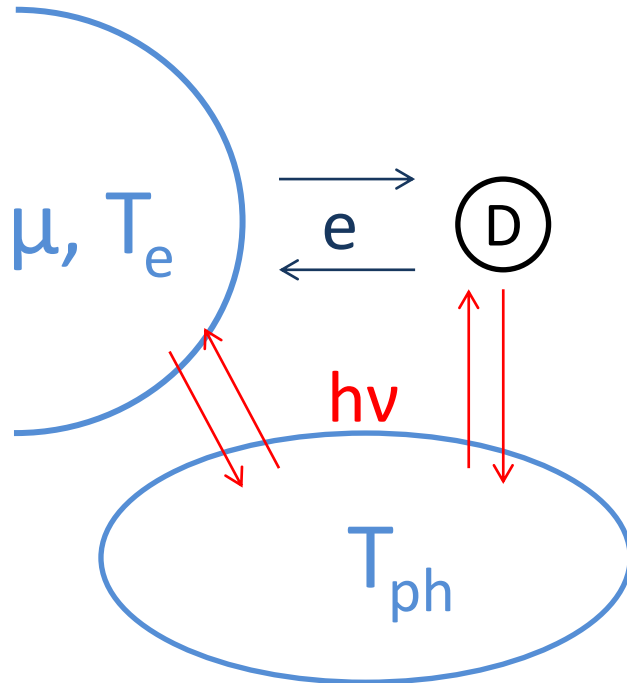
# Lādiņa pārnese kvantu sūkņos: kvantu punkta temperatūras ietekme

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Eiropas Savienības struktūrfondu projekta  
Nr. 2009/0216/1DP/1.1.1.2.0/09/APIA/VIAA/044  
„Datorzinātnes pielietojumi un tās saiknes ar kvantu fiziku” ietvaros

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# Small systems: Statistical ensembles



## Equilibrium

- microcanonical ensemble
- defined  $P_n$  and  $P(E)$

## Non-equilibrium

- unknown  $P_n(E, t)$
- solvable, but difficult

## Fast coupling to thermal bath

- $T_{dot} = T_{ph} = T_e$
- fast relaxation in the dot
- canonical ensemble
- $P_n(E, t) = P_n(t)P_{canon}(E, n)$
- unknown  $P_n(t)$
- solvable and easier

## Main assumptions:

- electron exchange with the lead ( $P_n(t)$ )
- energy relaxation in the dot is much faster than typical time between tunneling events (equilibrium probability distribution in the dot for fixed  $n$ )
- energy exchange with thermal bath ( $T_{everywhere} = \text{const}$ , canonical ensemble)

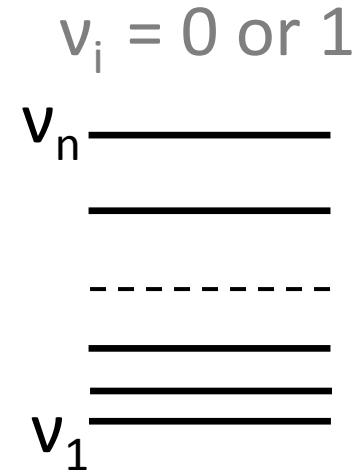
## Small systems: Kinetic equation

$$\frac{dP_n}{dt} = P_{n+1}W_{n+1}^- + P_{n-1}W_{n-1}^+ - P_nW_n^- - P_nW_n^+$$

# Small systems: Structure of the dot

## Constant interaction model

- electron adds only charging energy  $E_c$
- single-particle energy spectrum is not affected by any other interactions inside the dot
- $n$  independently occupied levels out of many



$$E_{full} = E_c(n) + \sum_m \epsilon_m v_m$$

$$\{v_m\} = \{0, 1, 0 \dots 1, 1\}$$

$$P_{canon}(E, n) = P_{eq}(\{v_m\}|n) = \frac{1}{Z_n} e^{-\frac{E_{full}(\{v_m\})}{kT}}$$

$$Z_n = e^{-\frac{F_n}{kT}}$$

- electrons tunnel independently

$$\Gamma_{full} = \sum_m \gamma_m^- v_m$$

## Small systems: Kinetic equation's coefficients

$$\frac{dP_n}{dt} = P_{n+1}W_{n+1}^- + P_{n-1}W_{n-1}^+ - P_nW_n^- - P_nW_n^+$$

$$f(\varepsilon) = \frac{1}{e^{\frac{\varepsilon-\mu}{kT}} + 1}$$

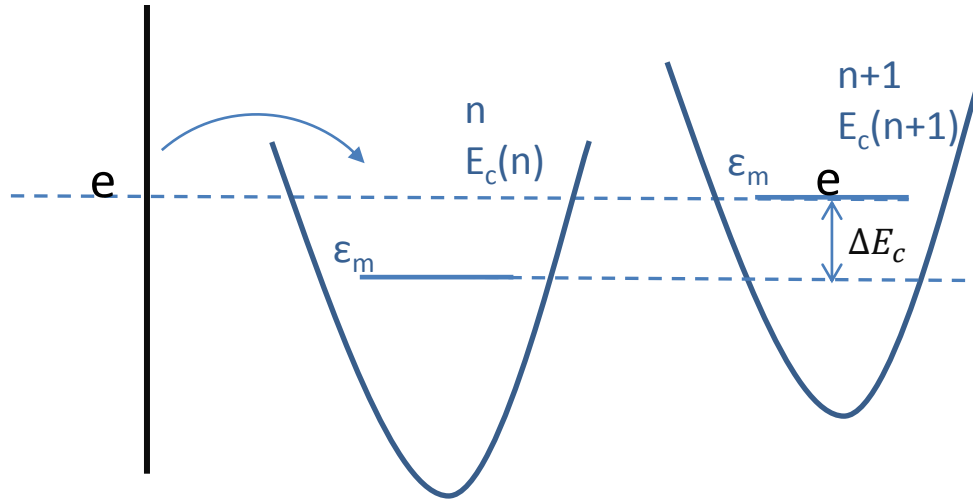
$$W_{n+1}^- = \sum_{\{v_m\}} P_{eq}(\{v_m\}|n+1) \sum_m v_m \gamma_m^-(n+1) [1 - f(\Delta E_c(n+1) + \varepsilon_m)]$$

$$W_n^+ = \sum_{\{v_m\}} P_{eq}(\{v_m\}|n) \sum_m (1 - v_m) \gamma_m^+(n) f(\Delta E_c(n+1) + \varepsilon_m)$$

$$W_{n-1}^+ = \sum_{\{v_m\}} P_{eq}(\{v_m\}|n-1) \sum_m (1 - v_m) \gamma_m^+(n-1) f(\Delta E_c(n) + \varepsilon_m)$$

$$W_n^- = \sum_{\{v_m\}} P_{eq}(\{v_m\}|n) \sum_m v_m \gamma_m^-(n) [1 - f(\Delta E_c(n) + \varepsilon_m)]$$

# Small systems: $\Delta E_c$



$$\Delta E_c(n+1) = E_c(n+1) - E_c(n)$$

$$E_c \propto n^2$$

$$\Delta E_c \propto n$$

## Small systems: Microreversibility

$$\gamma_m^+(n) = \gamma_m^-(n + 1)$$

$$W_{n+1}^- = \sum_{\{v_m\}} P_{eq}(\{v_m\}|n + 1) \sum_m v_m \gamma_m^-(n + 1) [1 - f(\Delta E_c(n + 1) + \varepsilon_m)]$$

$$W_n^+ = \sum_{\{v_m\}} P_{eq}(\{v_m\}|n) \sum_m (1 - v_m) \gamma_m^-(n + 1) f(\Delta E_c(n + 1) + \varepsilon_m)$$

$$W_{n-1}^+ = \sum_{\{v_m\}} P_{eq}(\{v_m\}|n - 1) \sum_m (1 - v_m) \gamma_m^-(n) f(\Delta E_c(n) + \varepsilon_m)$$

$$W_n^- = \sum_{\{v_m\}} P_{eq}(\{v_m\}|n) \sum_m v_m \gamma_m^-(n) [1 - f(\Delta E_c(n) + \varepsilon_m)]$$

# Small systems: Solution

## 1. Introduction

Applications of statistical mechanics to fermion systems with discrete spectrum, such as semiconductor quantum dots [1], naturally involve single-particle averages in statistical ensembles with fixed number of particles. In particular, the kinetic theory of tunneling [2, 3] through quantum dots with fast intra-dot electron relaxation involves average level occupation number,

$$\langle n_k \rangle = \frac{-1}{\beta} \frac{\partial Z_n}{\partial \epsilon_k} \quad (1)$$

in a Gibbs distribution of  $n$  independent fermions populating a set of single-particle energy levels  $\{\epsilon_k\}$  (enumerated by  $k = 0, 1, 2, \dots$ ). Here  $Z_n$  is the canonical partition function

$$Z_n = \sum_{\{n_k\}} \exp(-\beta \sum_k n_k \epsilon_k) \epsilon_k \zeta_{n-k}, \quad (2)$$

and  $\beta$  is the inverse thermodynamic temperature. For fermions, occupation numbers  $n_k$  in the sum (2) take values 0 and 1.

The behavior of  $\langle n_k \rangle$  is simple in two extreme limits of the typical level  $\Delta\epsilon$ . For  $\beta\Delta\epsilon \ll 1$  and large  $n$ , Exp. (1)-(2) reduce to the standard Fermi-Dirac distribution,

$$\langle n_k \rangle = f(\epsilon_k - \mu) = \frac{1}{1 + e^{\beta(\epsilon_k - \mu)}}. \quad (3)$$

Here  $\mu$  is the chemical potential determined by the normalization condition  $n = \sum_k f(\epsilon_k - \mu)$ . In the low temperature limit,  $\beta\Delta\epsilon \gg 1$ , most of the statistical weight in Eq. (2) is in the ground state (defined as  $n_k = 1$  for  $0 \leq k < n$  and  $n_k = 0$  otherwise). In this case it is common [4, 5] to take only one excited state into account resulting in a two-state Gibbs distribution which is equivalent to Eq. (3) for  $k = n-1$ ,  $n$  with  $\mu = (\epsilon_{n-1} + \epsilon_n)/2$  and  $\beta \rightarrow \beta^* = 2\beta$ . [2].

For finite  $\beta\Delta\epsilon$ , the average occupation number  $\langle n_k \rangle$ , deviates from Eq. (3) in a non-universal way which depends on the details of the energy spectrum [2, 6]. To the best of the author's knowledge, this crossover regime has not been studied analytically, presumably due to combinatorial explosion in the number of levels with comparable statistical weights.

In the paper we resolve the problem of exact evaluation of canonical occupation numbers  $\langle n_k \rangle$ , by providing a general formula which scales linearly in the number of levels and quadratically in the number of particles, Eqs. (8) and (10) below. We apply this general result to equilibrium spectrum,  $\epsilon_k = k\Delta\epsilon$ , and derive an exact formula for  $\langle n_k \rangle$ , in terms of polynomials in  $q = e^{-\beta\Delta\epsilon}$ , Eq. (13). In the limit of degenerate Fermi gas,  $n\Delta\epsilon \gg 1$ , these polynomials converge to partial theta function [7] which is involved in a number of combinatorial proofs [8, 9, 10] of Ramanujan's identities [11]. The exact result for the equilibrium spectrum can be approximated well by tailoring two standard Fermi-Dirac distributions (3) with different chemical potentials for holes and for particles,  $\mu_h = \epsilon_n$  and  $\mu_p = \epsilon_{n-1}$ , respectively. In the high and the low-temperature limits, this approximation converges to the asymptotically exact Fermi-Dirac and two-state Gibbs distributions, respectively, while at intermediate temperatures,  $\beta\Delta\epsilon < 1$ , particle-hole correlation effects due to fixed  $n$  result in finite deviations from the exact solution.

## 2. General expressions for fermion partition functions and the occupation numbers

Grand canonical partition function  $Y$  serves as a generating function for the canonical partition functions  $Z_n$ , if expanded power series of  $z = e^{\beta\mu}$ ,

$$Y(z) = \sum_{\{n_k\}} \exp(-\beta \sum_k n_k (\epsilon_k - \mu_0)) = 1 + \sum_{n=1}^{\infty} Z_n z^n, \quad (4)$$

$Y(z)$  is most conveniently calculated via its logarithm [12],

$$\ln Y(z) = \sum_k \ln(1 + ze^{-\beta\epsilon_k}) = \sum_{n=1}^{\infty} \frac{z^n}{n} \kappa_n, \quad (5)$$

where  $\kappa_n \equiv (-1)^{n+1}(n-1)!Z_n(\beta n)$ , and

$$Z_n(\beta) = \sum_{\{n_k\}} e^{-\beta \sum_k n_k \epsilon_k} \quad (6)$$

is the canonical partition function of a single particle.

Relation between  $n!Z_n$  and  $\kappa_n$  is the same as between the raw moments and the cumulants of a univariate probability distribution. The latter are connected by a recurrence relation [13],

$$n!Z_n = \kappa_n - \sum_{m=1}^{n-1} \binom{n-1}{m-1} \kappa_m (n-m)!Z_{n-m}, \quad (7)$$

which translates into

$$Z_n = \frac{1}{n} \sum_{m=1}^n (-1)^{m+1} Z_1(\beta m) \kappa_{n-m}. \quad (8)$$

We set  $Z_0 = 1$  identically.

Combining Eqs. (1), (4) and (5) gives the generating function for the occupation numbers,

$$\sum_{n=0}^{\infty} \langle n_k \rangle z^n = Y(z) + \frac{ze^{-\beta\epsilon_k}}{1 - ze^{-\beta\epsilon_k}}. \quad (9)$$

Expanding the r.h.s. in powers series in  $z$  gives

$$\langle n_k \rangle = \frac{1}{Z_n} \sum_{m=1}^n (-1)^{m+1} e^{-\beta m \epsilon_k} Z_{n-m}. \quad (10)$$

Equations (8) and (10) constitute our main general result.

## 3. Example: equilibrium spectrum

### 3.1. Exact finite- $n$ results: polynomials

For  $\epsilon_k = k\Delta\epsilon$ , the grand canonical partition function (5) can be expressed by an infinite product,

$$Y(z) = \prod_{k=0}^{\infty} (1 + q^k z) = (-z; q)_{\infty}. \quad (11)$$

where  $q = e^{-\beta\Delta\epsilon}$  and  $(\cdot; q)_{\infty}$  is the  $q$ -shifted factorial [14, 15].

Using generating theorem of Euler [16], formula 17.2.35) we can get the partition function directly from Eq. (4),

$$Z_n = \frac{q^{n(n+1)/2}}{(q; q)_{\infty}} \quad (12)$$

Applying Eq. (10), and transforming  $q$ -shifted factorials [15], formula 17.2.13), one gets

$$\langle n_k \rangle = 1 - p(k, n, q), \quad (13)$$

$$p(k, n, q) = \sum_{m=0}^k q^{m(m+1)/2} (q^{-n}; q)_{m+1} \quad (14)$$

$$= 1 - \sum_{m=1}^n \prod_{i=0}^{k-1} (q^{i+1} - q^{i+k+1}). \quad (15)$$

Equation (13) defines occupation numbers for  $n$  fermions populating equilibrium levels at equilibrium. It is clear from the explicit form (15) that  $p(k, n, q)$  is a Laurent polynomial (the product contains negative powers of  $q$  if  $k < n$ ). However, since  $0 \leq \langle n_k \rangle \leq 1$  for  $q = 0$  by definition (1), the negative powers of  $q$  must cancel, thus we conclude that  $p(k, n, q)$  is always an ordinary polynomial in  $q$  for  $n > 0, k \geq 0$ . This cancellation is not trivial and demands further mathematical investigation [16].

A number of recurrence formulae can be derived for  $p(k, n, q)$  [17], including a symmetry relation

$$q^k p(k, n, q) = q^n p(n, k, q). \quad (16)$$

Using (15) in the r.h.s. of (16) gives a sum of products with no negative powers of  $q$  at  $k < n$ .

### 3.2. Large- $n$ limit: $q$ -analog of Fermi-Dirac distribution

If  $n \gg \beta^{-1}$  then the Fermi gas is degenerate [12] and the limit of  $q^n \rightarrow 0$  is appropriate. For  $k \rightarrow \infty$ , and  $k - n = \text{const} \geq -1$  the polynomial sum in Eq. (15) becomes a geometric series which gives

$$\lim_{n \rightarrow \infty} p(k, n, q) = \theta(-q^{k-n+1}; q^{1/2}), \quad (17)$$

$$\theta(n, q) = \sum_{k=0}^{\infty} q^{n+k} q^{k^2} \quad (18)$$

partial theta function [7]. The partial theta function is famous for  $q$ -identities discovered by Ramanujan in his lost notebook [11]. These were later studied extensively [18, 7], including some recent proofs by Almkvist [8, 9, 10]. Using the symmetry relation (16) for  $k < n$ , gives hole complementary result:  $\lim_{n \rightarrow \infty} p(k, n, q) = 1 - \theta(-q^{k+1}; q^{1/2})$ ,  $0 \leq k < n$ .  $\lim_{n \rightarrow \infty} p(k, n, q) = \sum_{m=0}^k (-1)^m q^{m(m+1)/2}$  is an instance of false theta series [18] in [3, Chapter 14].

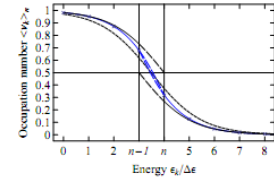


Figure 1. Comparison of different approximations for the canonical occupation numbers in a Fermi gas with equilibrium spectrum,  $n = 4$  and  $\beta\Delta\epsilon = 1$ . Crosses mark the exact values, dashed (blue) continuous line show the pairing of Fermi-Dirac distribution, Eq. (13), thin continuous line — substitution,  $f_k \rightarrow f$ , in Eq. (16), and short-dashed line — single Fermi-Dirac distribution, Eq. (3). The long-dashed line between  $\epsilon_{n-1}$  and  $\epsilon_n$  are extrapolations of the corresponding functions into the gap  $\mu_h < \epsilon < \mu_p$ .

In terms of level energies  $\epsilon_k$ , the occupation numbers in a canonical degenerate Fermi gas with constant levels spacing  $\Delta\epsilon$  can be written as

$$\lim_{n \rightarrow \infty} \langle n_k \rangle = \begin{cases} f_k(\epsilon_k - \mu - \Delta\epsilon/2), & \epsilon_k > \mu + \Delta\epsilon/2, \\ 1 - f_k(-\epsilon_k + \mu + \Delta\epsilon/2), & \epsilon_k < \mu - \Delta\epsilon/2, \end{cases} \quad (19)$$

where

$$f_k(\epsilon) = \theta(-e^{-\beta(\epsilon - \mu + \Delta\epsilon/2)}; q^{1/2}) q^{k^2} f(\epsilon). \quad (20)$$

and  $\mu = (\epsilon_n + \epsilon_{n-1})/2$ . The function defined in Eq. (19) can be considered a  $q$ -analog [14] of the standard Fermi-Dirac distribution (3) since  $\lim_{q \rightarrow 1} f_k(\epsilon) = f(\epsilon)$ .

Equation (19) expresses two essential deviations of canonical occupation numbers from Fermi-Dirac distribution. Firstly, the  $q$ -analog  $f_k$  is different from  $f$ . An approximation of substituting  $f_k \rightarrow f$  in Eq. (19) becomes exact both for  $q \rightarrow 1$  and for  $q \rightarrow 0$ . Numerically, we find maximal absolute deviation  $|f(\epsilon_k) - f_k(\epsilon_k)|$  of 0.0567 reached for  $k = n-1$  as  $\beta\Delta\epsilon = 0.752$ . For the two levels closest to the gap,  $k = n-1$ ,  $n$  approximating  $f_k \rightarrow f$  gives  $\langle n_{n-1} \rangle = 1 - \langle n_n \rangle = \exp(-\beta\Delta\epsilon/2) / (2 \cosh(\beta\Delta\epsilon/2))$  which is equivalent to two-state Gibbs approximation [2]. A comparison between the exact result (13), the large- $n$  limit (19) and a single Fermi-Dirac distribution is shown in Fig. 1 for  $n = 4$  and  $\beta\Delta\epsilon = 1$ .

Secondly, having the difference between  $f_k$  and  $f$ , Eq. (19) can be seen as a combination of two Fermi-Dirac distributions with different chemical potentials for particles,  $\mu_p = \mu - \Delta\epsilon/2 = \epsilon_{n-1}$ , and for holes,  $\mu_h = \mu + \Delta\epsilon/2 = \epsilon_n$ , respectively. This is precisely what is to be expected if one considers particle and hole excitations

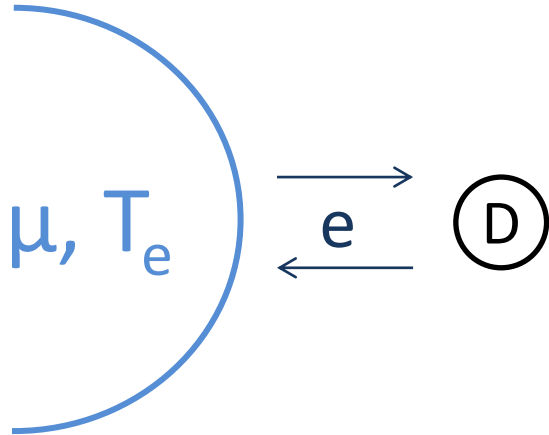


## Small systems: **Solution**

$$W_n^- = \frac{e^{\frac{\Delta E_c(n) - \mu}{kT}}}{Z_n} \left[ \sum_{m=0}^{n-1} Z_m (-1)^{n-m-1} \sum_k \frac{\gamma_k^-(n) e^{-\frac{\epsilon_k(n-m-1)}{kT}}}{e^{\frac{(\Delta E_c(n) + \epsilon_k - \mu)}{kT}} + 1} \right]$$

$$W_{n-1}^+ = \frac{1}{Z_{n-1}} \left[ \sum_{m=0}^{n-1} Z_m (-1)^{n-m-1} \sum_k \frac{\gamma_k^-(n) e^{-\frac{\epsilon_k(n-m-1)}{kT}}}{e^{\frac{(\Delta E_c(n) + \epsilon_k - \mu)}{kT}} + 1} \right]$$

# Small systems: Solution check



## Equilibrium

- microcanonical ensemble
- defined  $P_n$  and  $P(E)$

$$0 = P_{n+1}^{eq} W_{n+1}^- + P_{n-1}^{eq} W_{n-1}^+ - P_n^{eq} W_n^- - P_n^{eq} W_n^+$$

$$W_n^- = \frac{e^{\frac{\Delta E_c(n) - \mu}{kT}}}{Z_n} \left[ \sum_{m=0}^{n-1} Z_m (-1)^{n-m-1} \sum_k \frac{\gamma_k^-(n) e^{-\frac{\varepsilon_k(n-m-1)}{kT}}}{e^{\frac{(\Delta E_c(n) + \varepsilon_k - \mu)}{kT}} + 1} \right]$$

$$W_{n-1}^+ = \frac{1}{Z_{n-1}} \left[ \sum_{m=0}^{n-1} Z_m (-1)^{n-m-1} \sum_k \frac{\gamma_k^-(n) e^{-\frac{\varepsilon_k(n-m-1)}{kT}}}{e^{\frac{(\Delta E_c(n) + \varepsilon_k - \mu)}{kT}} + 1} \right]$$

$$Z_n = e^{-\frac{F_n}{kT}}$$

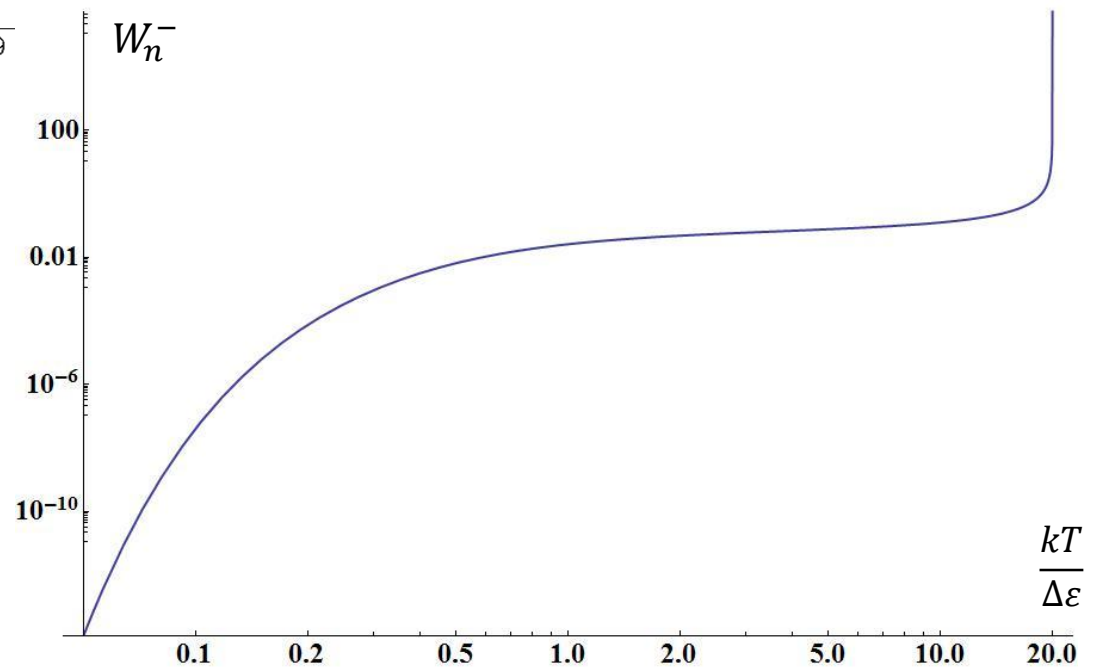
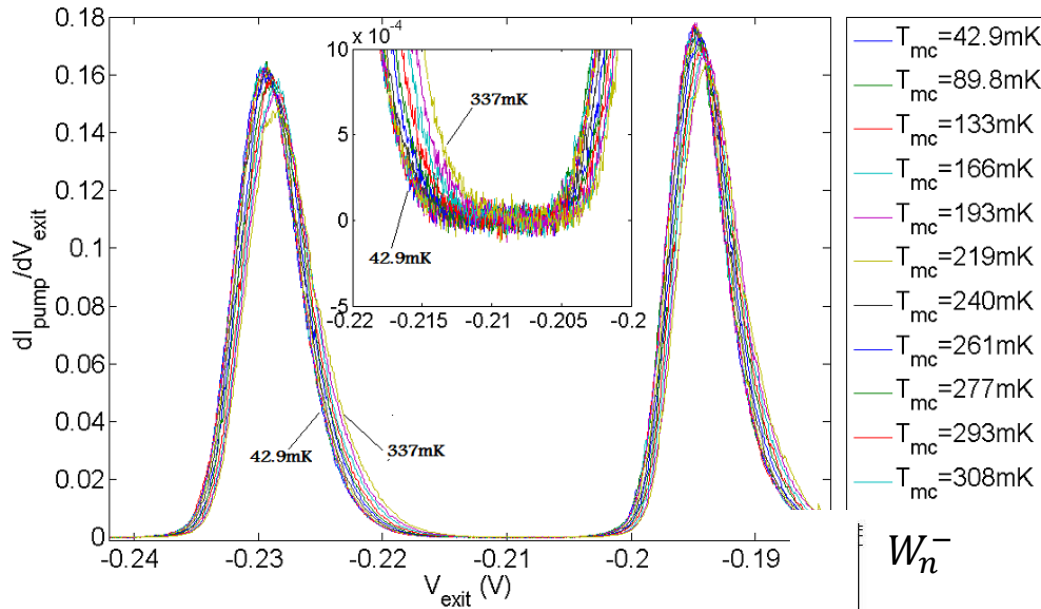
$$P_n^{eq} W_n^- = P_{n-1}^{eq} W_{n-1}^+$$

$$\frac{P_n^{eq}}{P_{n-1}^{eq}} = \frac{W_{n-1}^+}{W_n^-} = \frac{1}{Z_{n-1}} \frac{Z_n}{e^{\frac{\Delta E_c(n) - \mu}{kT}}}$$

$$= \frac{e^{-\frac{F_n}{kT} - \frac{E_c(n)}{kT} + \frac{\mu n}{kT}}}{e^{-\frac{F_{n-1}}{kT} - \frac{E_c(n-1)}{kT} + \frac{\mu(n-1)}{kT}}}$$

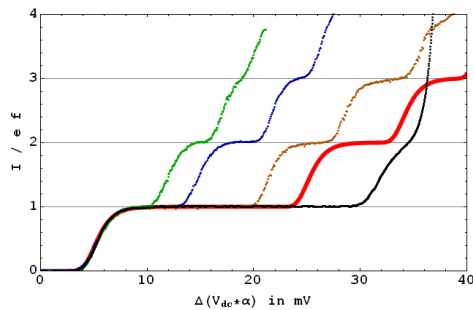
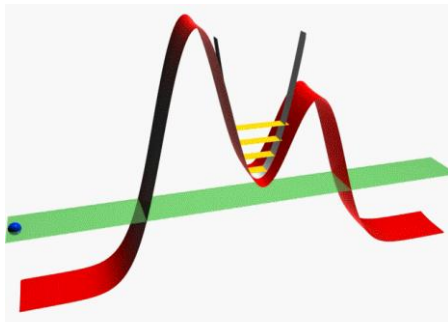
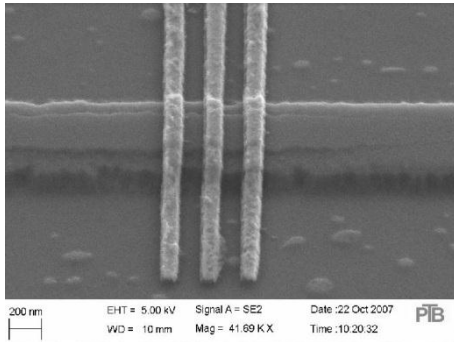
microcanonical!

# Small systems: Temperature in electron pumps

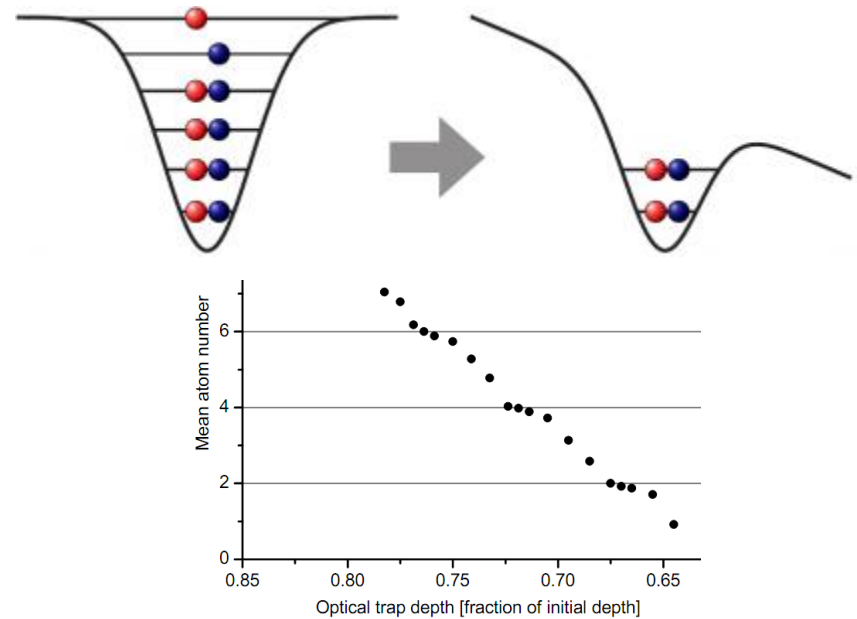
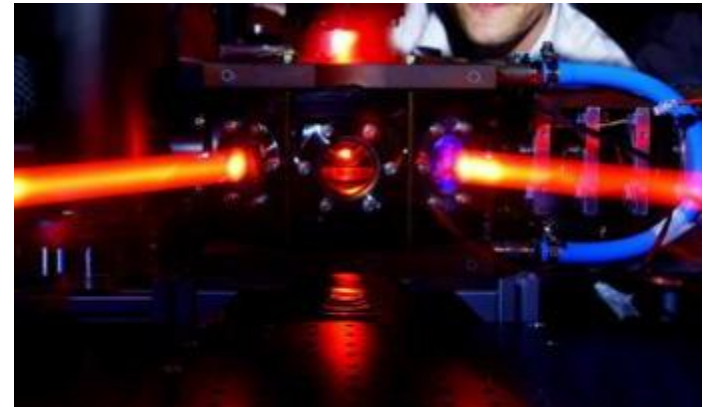


# Small systems: Examples

## Electron pumps



## Ultracold fermion gases



L. Fricke, F. Hohls, P. Mirovsky, C. Leicht, B. Kaestner and others „Measurements of two sequential quantized-charge pumps“, Phys.Rev.B (2011)

F. Serwane, T. Lompe, T.B. Ottenstein and others “Deterministic Preparation of a Tunable Few-Fermion System”, Science (2011)