LATVIJAS UNIVERSITATE

UNIVERSITY OF LATVIA

EIROPAS SOCIĀLAIS FONDS

EIROPAS SAVIENĪBA

IEGULDĪJUMS TAVĀ NĀKOTNĒ

ESF projekts "*Datorzinātnes lietojumi un tās saiknes ar kvantu fiziku*"
Nr. 2009/0216/1DP/1.1.1.2.0/09/APIA/VIAA/044

Fermī sadalījuma vispārinājums kvantu sistēmām ar diskrētu spektru

Vjačeslavs Kaščejevs, LU DF

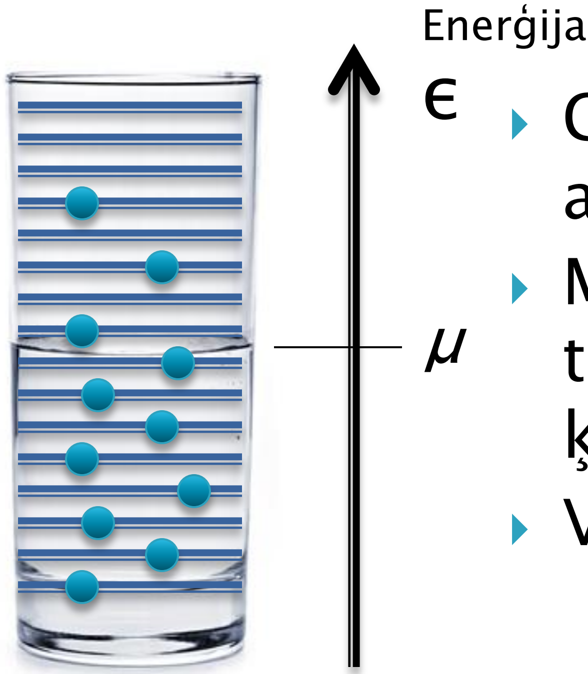
LU 70. konference

2012. gada 3. februārī

Fermionu statistika

Enrico Fermi
(1901–1954)

- Fermioni pakļaujas Pauli principam



T=  vai 

- Galīga kvantu sistēma ar diskrētu spektru $\{\varepsilon_k\}$
- Mikrokanoniskais ansamblis ar tempartūru T un ķīmisko potenciālu μ
- Vidējais daļiņu skaits līmenī ϵ :

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

Fermī funkcija

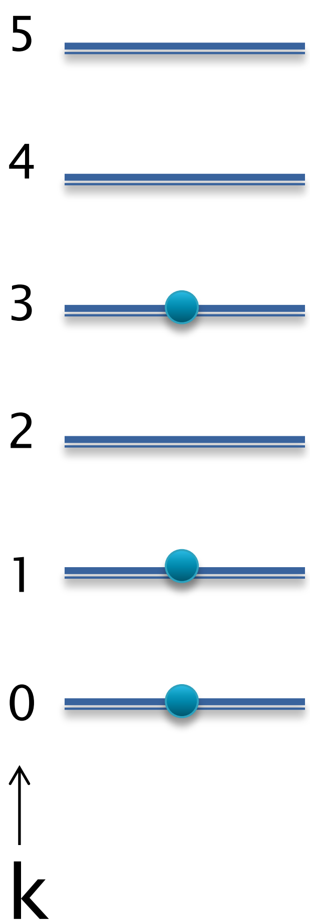
- Līmeņu apdzīvotības ir statistiski neatkarīgas

I. Vispārīgs formulējums

- Sistēma:
  - Ideālā kvantu gāze ar diskrētu spektru $\{\varepsilon_k\}$
  - Termodinamiskais līdzsvars ar temperatūru T,
  - **Kanoniskais** ansamblis:
    - daļiņu skaits n ir fiksēts

- Jautājums:
  - Kāda ir varbūtība tam, ka k-jā līmenī ir daļiņa?

No fizikas uz kombinatoriku



- Mikrostāvokli raksturo "bitu" virkne:

$$\{\nu_k\} = \{1, 1, 0, 1, 0, 0, \ldots\}$$

- Kanoniskā ansambļa ierobežojums:

$$\sum_k \nu_k = n$$

- Vidējais pēc Gibsa sadalījuma:

$$\langle \nu_k \rangle_n = \frac{1}{Z_n} \sum_{\{\nu_k\}}^{(n)} \nu_k \exp\Big(-\beta \sum_k \nu_k \epsilon_k\Big)$$

$$Z_n = \sum_{\{\nu_k\}}^{(n)} \exp\Big(-\beta \sum_k \nu_k \epsilon_k\Big)$$

Vispārīgā atbilde

VK, arXiv:1110.6264

$$\boxed{\langle \nu_k \rangle_n = \frac{1}{Z_n} \sum_{m=1}^{n} (-1)^{m+1} e^{-\beta m \epsilon_k} Z_{n-m}}$$

$\beta^{-1} = kT$

$$Z_n = \frac{1}{n} \sum_{m=1}^{n} (-1)^{m+1} \underbrace{Z_1(\beta m)}_{Z_1(\beta') = \sum_k e^{-\beta' \epsilon_k}} Z_{n-m}$$

$$Z_{\mathcal{N}} = e^{-F_{\mathcal{N}}/T} = \frac{e^{-\beta E_0}}{N_{sp}} \sum_{m=1}^{N_{sp}} \prod_{i=1}^{N_{sp}} (1 + e^{-\beta|E_i - \mu|} e^{i\sigma_i \phi_m}), \tag{140a}$$

$$\langle n_\lambda \rangle_{\mathcal{N}} = \frac{e^{-\beta E_0}}{N_{sp} Z_{\mathcal{N}}} \sum_{m=1}^{N_{sp}} \left[\prod_{i=1}^{N_{sp}} (1 + e^{-\beta|E_i - \mu|} e^{i\sigma_i \phi_m}) \right] \times \frac{1}{1 + e^{\beta(E_\lambda - \mu)} e^{i\phi_m}}, \tag{140b}$$

where the quadrature points are $\phi_m = 2\pi m / N_{sp}$ (N_{sp} is the number of single-particle states), and $E_0 = \Sigma_i E_i$. The

← Ormand et al, Phys. Rev .C (1997)

Izvedums

$$\langle \nu_k \rangle_n = \frac{1}{Z_n} \sum_{\{\nu_k\}}^{(n)} \nu_k \exp\Big(-\beta \sum_k \nu_k \epsilon_k\Big)$$

$$Z_n = \sum_{\{\nu_k\}}^{(n)} \exp\Big(-\beta \sum_k \nu_k \epsilon_k\Big)$$

$$\langle \nu_k \rangle_n = \boxed{\frac{-1}{\beta Z_n} \frac{\partial Z_n}{\partial \epsilon_k}}$$

$$Y = \sum_{\{\nu_k\}} \exp\Big(-\beta \sum_k \nu_k (\epsilon_k - \mu)\Big)$$

$$Y = 1 + e^{\beta\mu \cdot 1} \sum_{\nu_m}^{(1)} e^{-\beta \sum \nu_k \epsilon_k} + e^{\beta\mu}$$

$$Y = 1 + \sum_{n=1}^{\infty} Z_n z^n$$

$$Y = \sum_{\{\nu_k\}} \prod_k \exp\Big(-\beta \nu_k (\epsilon_k - \mu)\Big) =$$

$$\ln Y = \boxed{\sum_k \ln(1 + z e^{-\beta \epsilon_k})}$$

$$\frac{\partial \ln Y}{\partial \epsilon_k} = \frac{(-\beta) z e^{-\beta \epsilon_k}}{1 + z e^{-\beta \epsilon_k}} = \frac{1}{Y} \frac{\partial Y}{\partial \epsilon_k} = \frac{1}{Y} \sum_{n=1}^{\infty} \frac{\partial Z_n}{\partial \epsilon_k} z^n$$

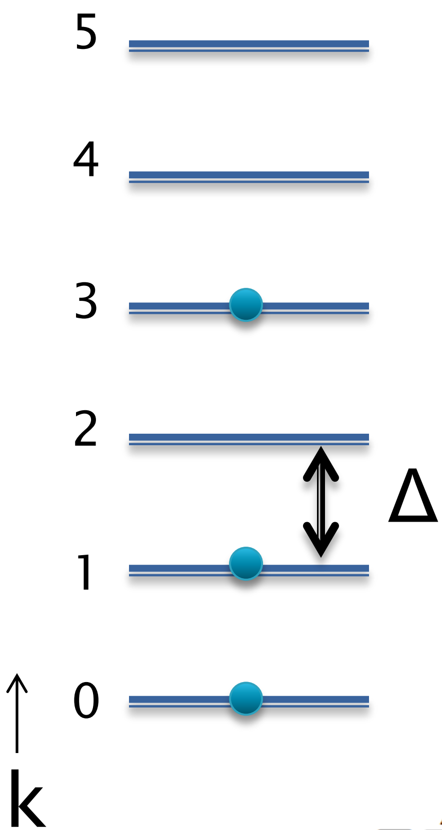
$$\sum_{n=1}^{\infty} \langle \nu_k \rangle_n Z_n z^n = Y(z) \frac{z e^{-\beta \epsilon_k}}{1 + z e^{-\beta \epsilon_k}}$$

$$\langle \nu_k \rangle_n = \boxed{\frac{1}{Z_n} \sum_{m=1}^{n} (-1)^{m+1} e^{-\beta m \epsilon_k} Z_{n-m}}$$

$$n = \frac{1}{Z_n} \sum_{m=1}^{n} (-1)^{m+1} \underbrace{\sum_k e^{-\beta m \epsilon_k}}_{Z_1(\beta m)} Z_{n-m}$$

$$Z_n = \boxed{\frac{1}{n} \sum_{m=1}^{n} (-1)^{m+1} Z_1(\beta m) Z_{n-m}}$$

II. Speciālgadījums



- Aplūkojam ekvidistantu spektru

$$\epsilon_k = k\Delta$$

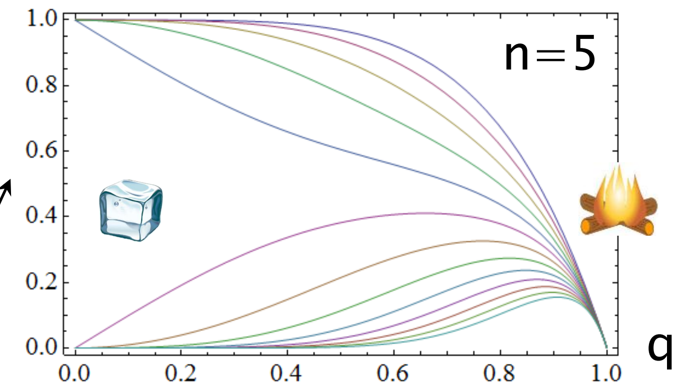
- Atbilde:

$$\begin{aligned}\langle \nu_k \rangle_n &= 1 - p(k,n;q)\ , \\ p(k,n;q) &\equiv \sum_{m=0}^{n} q^{m(k+1)} (q^{-n};q)_m \\ &= 1 + \sum_{m=1}^{n} \prod_{l=0}^{m-1} \left(q^{k+1} - q^{l+k-n+1}\right)\end{aligned}$$

$$q \equiv e^{-\frac{\Delta}{kT}}$$

Noslēpumainie polinomi

$$\boxed{p(k,n) \equiv 1 + \sum_{m=1}^{n} \prod_{l=0}^{m-1} \left(q^{k+1} - q^{l+k-n+1}\right)}$$

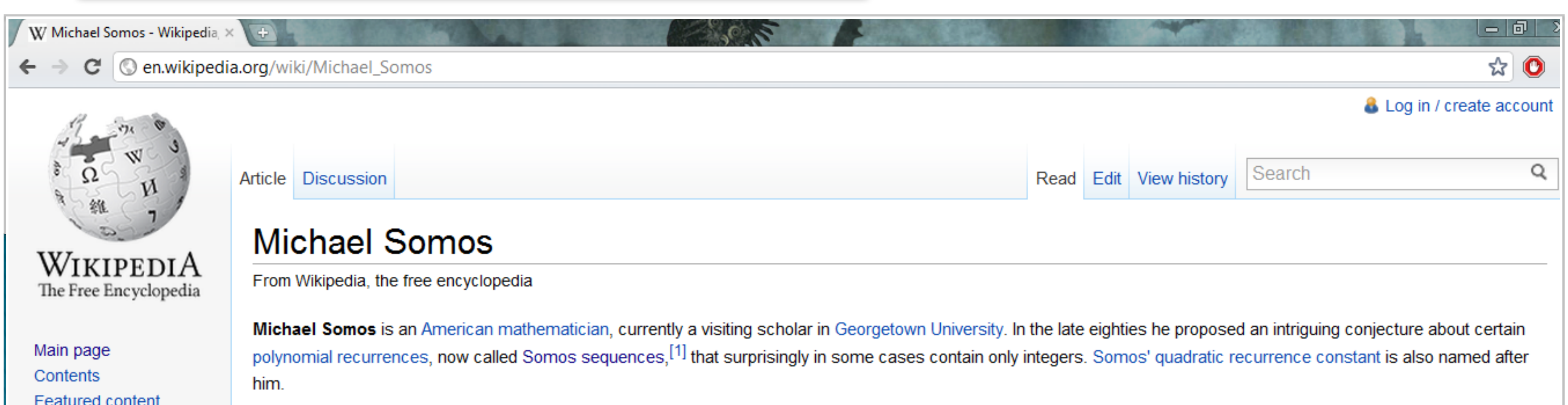


$$\langle \nu_k \rangle_n = 1 - p(k,n)$$

- Kāpēc tie ir polinomi?

$$p(0,2) = 1 + \left(q - \frac{1}{q}\right) + \left(q - \frac{1}{q}\right)(q-1) = q^2$$

- $\boxed{q^k p(k,n) = q^n p(n,k)}$ [Juris Smotrovs]



III. Fermī funkcijas vispārinājums

- ... ekvidistantam spektram.
- Apskatām lielu daļiņu skaitu (bet galīgu Δ):

$$\lim_{n\to\infty} p(n,k) = \begin{cases} \theta(-q^{k-n+1/2}, q^{1/2}), & k \geq n \\ 1-\theta(-q^{n-k-1/2}, q^{1/2}), & k < n \end{cases}$$

$$\boxed{f_q(\epsilon) \equiv \theta(-e^{-\beta\epsilon}, q^{1/2}) \overset{q\to 1}{=} f(\epsilon)}$$

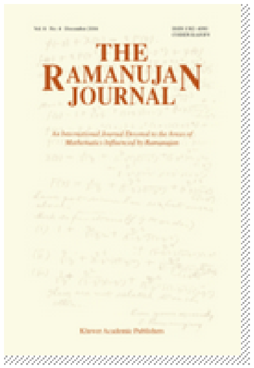
Rogers–Ramanujan
partial theta function $\Theta(a,q)$

We conclude our discussion of combinatorial proofs by offering a few remarks about an identity

$$\sum_{n=0}^{\infty} a^n q^{n^2} = \sum_{n=0}^{\infty} \frac{(-q;q)_{n-1} a^n q^{n(n+1)/2}}{(-aq^2;q^2)_n} \tag{3.4}$$

found on page 28 in Ramanujan's lost notebook [57]. (The claims that we

Indijas ģēnijs: Srinivasa Ramanujan



The Ramanujan Journal

An International Journal Devoted to the Areas of Mathematics Influenced by Ramanujan

Editor-in-Chief: Krishnaswami Alladi

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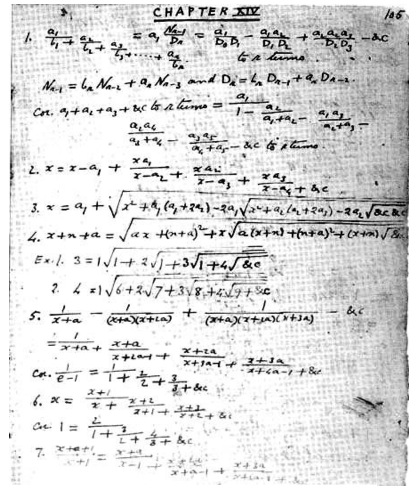


(1887-1920)

1. Introduction

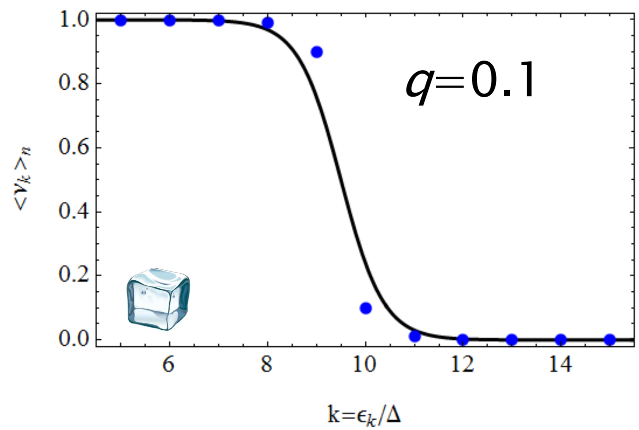
G. E. Andrews' discovery in 1976 of Ramanujan's lost notebook [19] can probably be regarded as one of the most exciting finds ever in mathematics. The lost notebook, which was hidden in a box containing papers from the late G. N. Watson's estate, is a handwritten manuscript of well over a hundred pages of hardly

We conclude our discussion of combinatorial proofs by offering a few remarks about an identity

$$\sum_{n=0}^{\infty} a^n q^{n^2} = \sum_{n=0}^{\infty} \frac{(-q;q)_{n-1} a^n q^{n(n+1)/2}}{(-aq^2;q^2)_n} \tag{3.4}$$

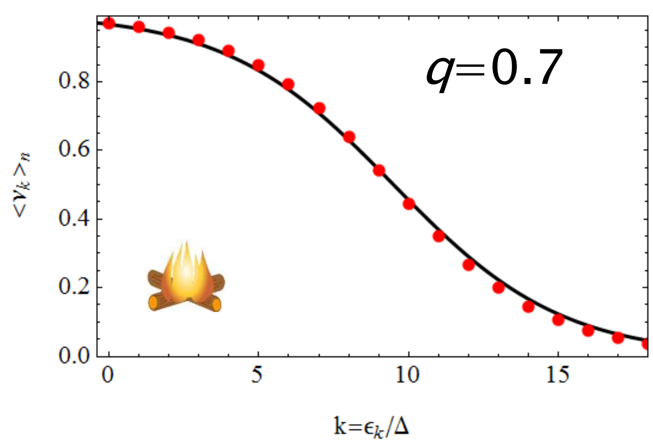
found on page 28 in Ramanujan's lost notebook [57]. (The claims that we

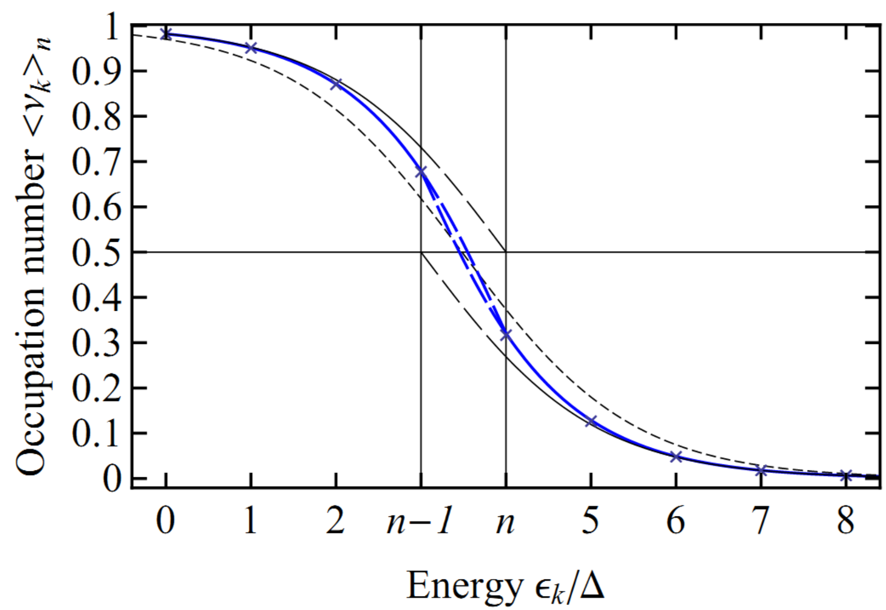
Fermī funkcijas vispārinājums



$$\lim_{n\to\infty}\langle \nu_k\rangle_n = \begin{cases} f_q(\epsilon_k-\mu+\Delta/2), & \epsilon_k>\mu+\Delta/2\,, \\ 1-f_q(-\epsilon_k+\mu+\Delta/2), & \epsilon_k<\mu-\Delta/2\,, \end{cases}$$

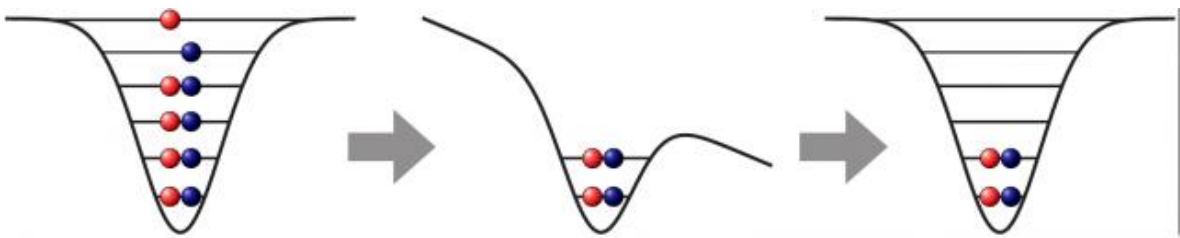
$$\boxed{f_q(\epsilon)\equiv\theta(-e^{-\beta\epsilon},q^{1/2}) \overset{q\to 1}{=} f(\epsilon)}$$



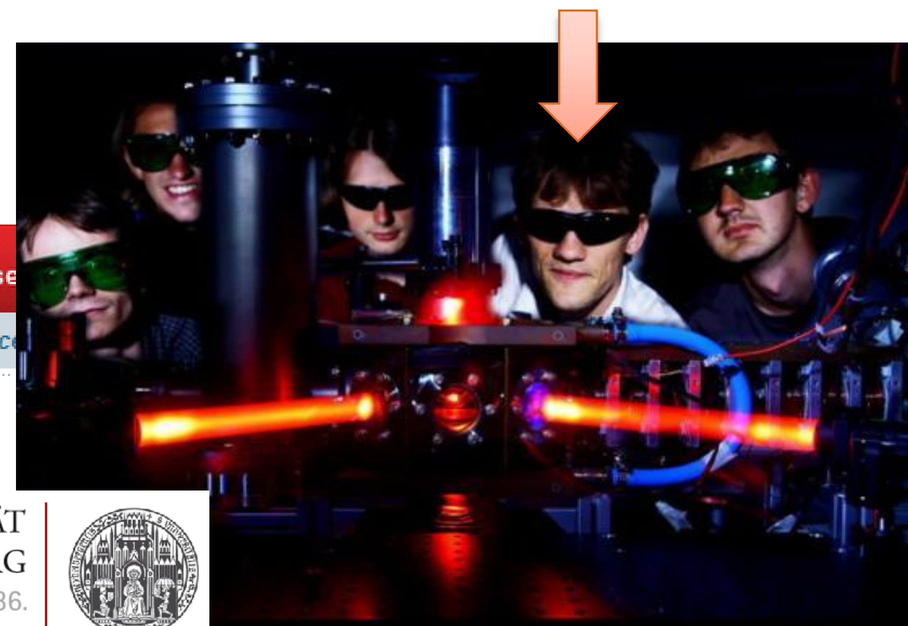


$$q\equiv e^{-\frac{\Delta}{kT}}$$

Realizācija aukstajos atomos



Selim Jochim



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Zukunft. Seit 1386.

REPORT

Deterministic Preparation of a Tunable Few-Fermion System

F. Serwane[1,2,3,*,†], G. Zürn[1,2,†], T. Lompe[1,2,3], T. B. Ottenstein[1,2,3,‡], A. N. Wenz[1,2], and S. Jochim[1,2,3]

Paldies!

physics.stackexchange.com/questions/13711/combinatorial-sum-in-a-problem-with-a-fermi-gas

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Combinatorial sum in a problem with a Fermi gas

4

I'm solving a problem involving a Fermi gas. There is a specific sum I cannot figure my way around.

A set of equidistant levels, indexed by $m = 0, 1, \ldots$, is populated by spinless fermions with population numbers $\nu_m = 0$ or 1. I need to compute the following sum over the set of all possible configurations $\{\nu_l\}$:

$$Q(\beta, \beta_c) = \sum_{\{\nu_l\}} \sum_l \prod_m \exp(\beta_c l \nu_l - [\beta m + i\phi]\nu_m).$$

Any hints on how to deal with this are appreciated. This is not homework, it is a research problem.

It is known that $\beta > 0$, $\beta_c > 0$, and $\phi \in [0; 2\pi]$.

EDIT: corrected with the complex phase (the sum is coming from a generating function)

mathematical-physics mathematics fermions

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edited **Aug 19 at 7:40**

asked **Aug 18 at 14:18**

Slaviks

708 11

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