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Mathematical Statistical Physics

MATHEMATISCHES INSTITUT

Solution Sketch of the math part of the Exam

| Family Name: | | F | First name: | | | |
|--------------|-------|---------------------|-----------------|----------|--|--|
| Student ID: | | | | | | |
| Program: | □ TMP | □ M.Sc. Mathematics | □ M.Sc. Physics | □ Other: | | |

Please switch off your mobile phone; place your identity and student ID cards on the table so that they are clearly visible.

Please do not write with the colours red or green. Write on every page your family name and your first name.

Write your solutions on the page marked with the appropriate problem number. If you run out of space, use the empty pages at the end of the examination paper ensuring that each problem is clearly marked.

Please make sure to submit only one solution for each problem; cross out everything that should not be graded. Solutions will be only accepted if all steps are mathematically precise and explained in a comprehensible way.

By entering a pseudonym (e.g. the last four digits of your student ID number) in the appropriate box on the left at the bottom of this page you will give your permission to the publication of your results on the lecture's homepage.

You have **180 minutes** in total to complete this examination.

Good luck!

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Problem 1. ...

Problem 2. ...

Problem 3.

[2+3+2+3 points]

Give brief and precise answers to the following short questions.

- a) Let $N \in \mathbb{N}$ be even. N classical particles can each be either in state 1 or in state 2. A particle in state 1 has energy E and one in state 2 has energy 2E. Compute the Boltzmann entropy of the macrostate M_1 with total energy $\frac{3}{2}NE$ and of the macrostate M_2 with total energy NE.
- b) Assume we have 1000 particles which are each in one of 2 boxes. The probability for each particle to be in the right box is $\frac{1}{3}$, independently of each other. Use Chebyshev's inequality to give an upper bound for the probability that the fraction of particles in the left box is smaller than $\frac{1}{2}$. Then state how one could improve this bound (A keyword suffices).
- c) Consider the dynamical system $(\Omega, \mathcal{B}(\Omega), \mu, T)$ given by the free Hamiltonian evolution T of an ideal gas of N particles on a torus T^3 , the microcanonical (Lebesgue) measure μ on Ω and $\Omega = (T^3)^N \times \mathcal{E}$, where

$$\mathcal{E} = \{ (p_1, ..., p_{3N}) \in \mathbb{R}^{3N} | \sum_{i=1}^{3N} \frac{p_i^2}{2m} = E \}$$

is the energy shell. Is this system ergodic? Prove your answer!

d) In which dimensions does Bose-Einstein condensation occur for a gas of free bosons with a relativistic dispersion, i.e. one-particle Hamiltonian $\mathcal{H} = \sqrt{-\Delta}$? Give a short argument, not a rigorous proof.

Solution of a) If n particles are in state 1, the number of possibilities is given by the binomial coefficient $W = \frac{N!}{n!(N-n)!}$. Moreover, the total energy is nE + 2(N-n)E = 2NE - nE. In macrostate M_1 , this implies $n = \frac{N}{2}$, so $S = k_B \ln(W) = k_B \ln\left(\frac{N!}{(N/2)!(N/2)!}\right) = k_B \ln N! - 2k_B \ln(N/2)!$. In macrostate M_2 , all particles are in state 1, so W = 1 and S = 0.

Solution of b) The particles can be referred to by random variables $X_i : \Gamma \to \{0, 1\}$ (1 for being in the right box) which are i.i.d. with Bernoulli distribution, $\mathbb{E}(X_i) = p = \frac{1}{3}$, $\operatorname{Var}(X_i) = pq = \frac{2}{9}$. The variable $\bar{X} = \frac{1}{N} \sum_{k=1}^{N} X_k$ then has $\mathbb{E}(\bar{X}) = p = \frac{1}{3}$, $\operatorname{Var}(\bar{X}) = \frac{pq}{N} = \frac{2}{9N}$. Then we use Chebyshev:

$$\mathbb{P}(\operatorname{left} < \frac{1}{2}) \le \mathbb{P}(|\bar{X} - \frac{1}{3}| > \frac{1}{6}) \le \frac{2}{9N \cdot \frac{1}{6^2}} = \frac{8}{1000} = \frac{1}{125}$$

A better bound can be obtained by using higher moments in the Markov inequality.

Solution of c) This system is not ergodic. The momentum components of each particle cannot change during the time evolution, so the set $A := \{(q_1, ..., q_{3N}, p_1, ..., p_{3N}) \in \Omega | a \leq p_1 \leq b\}$ is invariant, but has for suitable choice of a and b a measure $0 < \mu(A) < 1$, contradicting ergodicity.

Solution of d) On the exercise sheet, we have seen that the relative occupation number in the ground state is bounded from below as follows:

$$\lim_{n \to \infty} \frac{n_0}{N} \ge 1 - C \int d^d k \frac{e^{-\beta E(k)}}{1 - e^{-\beta E(k)}}$$

In our case, we have $E(k) \sim |k|$. The ground state is macroscopically occupied iff the following integral converges:

$$\int d^d k \frac{e^{-\beta|k|}}{1 - e^{-\beta|k|}} \sim C \int_0^\infty dx x^{d-1} \frac{e^{-\beta x}}{1 - e^{-\beta x}}$$

At ∞ , the exponential drops fast enough so there is never a problem. In a vicinity of 0, the integrand behaves like x^{d-2} . Therefore, the integral converges iff $d \ge 2$. This means we expect BEC in $d \ge 2$.

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Problem 4.

Consider the dynamical system given by the probability space $(\Omega, \mathcal{B}(\Omega), \mathbb{P})$ and a continuous map $T : \Omega \to \Omega$ that preserves \mathbb{P} .

[5+5 points]

a) Prove that ergodicity of this dynamical system is equivalent to the following property: For all $A \in \mathcal{B}(\Omega)$ with $\mathbb{P}(A) > 0$, we have

$$\mathbb{P}\left(\bigcup_{k=2016}^{\infty} T^{-k}(A)\right) = 1$$

b) Now suppose Ω is a compact metric space, \mathbb{P} is ergodic and satisfies $\mathbb{P}(U) > 0$ for every non-empty open set U. Prove that almost every $x \in \Omega$ has a dense orbit. *Hint: Use the well-known fact that a compact metric space has a countable base for its topology. (Recall that a base B for a topology is a collection of open sets such that any open set can be written as a union of sets in B.)*

Solution of a) Direction \Leftarrow : Let $A \in \mathcal{A}$ be invariant and $\mathbb{P}(A) > 0$. Then, $\mathbb{P}(\bigcup_{k=0}^{\infty} T^{-k}(A)) = \mathbb{P}(A) = 1$, which shows ergodicity.

Direction \Rightarrow : Let $A \in \mathcal{A}$ with $\mathbb{P}(A) > 0$. Call $B := (\bigcup_{k=2016}^{\infty} T^{-k}(A))$, then $T^{-1}(B) = T^{-1}(\bigcup_{k=2016}^{\infty} T^{-k}(A)) = \bigcup_{k=2017}^{\infty} T^{-k}(A)$. So we have $T^{-1}(B) \subset B$. Also, by measure invariance, $\mathbb{P}(T^{-1}(B)) = \mathbb{P}(B)$, which implies

$$\mathbb{P}(B \setminus T^{-1}(B)) = \mathbb{P}(B) - \mathbb{P}(T^{-1}(B)) = 0.$$

So B is invariant up to a set of measure zero and has positive measure, which implies $\mathbb{P}(B) = 1$, which is the claim. QED.

Solution of b) It is known (given) that a compact metric space has a countable base for its topology. Let's call this $(U_n)_{n \in \mathbb{N}}$. Since any open set is a union of base elements, a point $x \in X$ has dense orbit O(x) iff $O(x) \cap U_n \neq \emptyset \ \forall n \in \mathbb{N}$. Therefore, it has no dense orbit if there exists $n \in \mathbb{N}$ with $O(x) \cap U_n = \emptyset$. So we may write the set of all x which have no dense orbits as follows:

$$A := \{x \in X | O(X) \text{ not dense}\} = \bigcup_{n \in \mathbb{N}} \left(\bigcup_{k=0}^{\infty} T^{-k}(U_n)\right)^c$$

The second equality also establishes that A is measurable. By ergodicity and the property $\mathbb{P}(U_n) > 0$, it follows that $\mathbb{P}(\bigcup_{k=0}^{\infty} T^{-k}(U_n)) = 1$. Therefore,

$$\mathbb{P}(A) \le \sum_{n=0}^{\infty} \mathbb{P}\left(\left(\bigcup_{k=0}^{\infty} T^{-k}(U_n)\right)^c\right) = \sum_{n=0}^{\infty} 0 = 0.$$

Therefore, $\mathbb{P}(A) = 0$ and almost every $x \in X$ has a dense orbit. QED.

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Problem 5.

In the derivation of effective equations like the Hartree equation, one encounters terms like the following:

$$T := \langle \psi, q_1 q_2 V(x_1 - x_2) p_1 p_2 \psi \rangle.$$

Here, $\psi \in L^2(\mathbb{R}^{3N})$ is a normalized bosonic (symmetric) wave function, V is a real-valued function that satisfies $||V||_{\infty} < \infty$, $p_j = |\varphi\rangle \langle \varphi|(x_j)$ is the projector on the one-particle wave function $\varphi \in L^2(\mathbb{R}^3)$ in the x_j -coordinate and $q_j = 1 - p_j$. We define

$$\alpha(\psi) := \langle \psi, q_1 \psi \rangle \,.$$

a) Prove that there is $C \in \mathbb{R}$ such that

$$|T| \le C\left(\frac{1}{N} + \alpha(\psi)\right).$$

b) In the derivation of effective equations, one wants to show that the full N-particle wave function ψ_t stays close to a product of one particle wave functions φ_t . Explain by means of a simple example why closeness in the sense of L^2 -norm is usually a too strong requirement. Which notion of closeness can be used instead?

Solution of a) Abbreviation: $V_{jk} = V(x_j - x_k)$.

$$\begin{aligned} |T| &= |\langle \psi, q_1 q_2 V_{12} p_1 p_2 \psi \rangle | \\ &= \left| \frac{1}{N-1} \left\langle q_1 \psi, \sum_{j=2}^N q_j V_{1j} p_1 p_j \psi \right\rangle \right| \\ &\stackrel{\text{Cauchy Schwarz}}{\leq} \frac{1}{N-1} ||q_1 \psi|| ||\chi|| \end{aligned}$$

where $\chi := \sum_{j=2}^{N} q_j V_{1j} p_1 p_j \psi$. Note that $||q_1 \psi|| = \sqrt{\langle q_1 \psi, q_1 \psi \rangle} = \sqrt{\alpha}$.

$$\begin{aligned} \|\chi\|^{2} &= \sum_{j,k=2}^{N} \langle \psi, p_{j} p_{1} V_{1j} q_{j} q_{k} V_{1k} p_{1} p_{k} \psi \rangle \\ &= |\sum_{j \neq k} \langle \psi, p_{j} p_{1} V_{1j} q_{j} q_{k} V_{1k} p_{1} p_{k} \psi \rangle + \sum_{k=2}^{N} \langle \psi, p_{k} p_{1} V_{1k} q_{k} V_{1k} p_{1} p_{k} \psi \rangle | \\ &= |\sum_{j \neq k} \langle q_{k} \psi, p_{j} p_{1} V_{1j} V_{1k} p_{1} p_{k} q_{j} \psi \rangle + \sum_{k=2}^{N} \langle \psi, p_{k} p_{1} V_{1k} q_{k} V_{1k} p_{1} p_{k} \psi \rangle | \\ &\leq (N-1)^{2} |q_{1} \psi|^{2} |p_{2} p_{1}|_{\text{op}}^{2} |V|_{\text{op}}^{2} + (N-1) |q_{1}|_{\text{op}} |p_{2} p_{1}|_{\text{op}}^{2} |V|_{\text{op}}^{2} \\ &\leq (N-1)^{2} |V|_{\infty}^{2} \alpha + (N-1) |V|_{\infty}^{2} \end{aligned}$$

Therefore,

$$|T| \leq \frac{1}{N-1} \sqrt{\alpha} \left[(N-1)^2 |V|_{\infty}^2 \alpha + (N-1) |V|_{\infty}^2 \right]^{\frac{1}{2}}$$
$$\leq \frac{\sqrt{\alpha}}{N-1} \left[(N-1) |V|_{\infty} \sqrt{\alpha} + \sqrt{(N-1)} |V|_{\infty} \right]$$
$$\leq C_1 \alpha + C_2 \frac{1}{\sqrt{N}} \sqrt{\alpha} \leq C \left(\frac{1}{N} + \alpha \right)$$

[7 + 3 points]

Here we used the facts that

$$\sqrt{a+b} \le \sqrt{a} + \sqrt{b}$$

as well as

$$2ab \le a^2 + b^2.$$

Solution of b) We want to express $\psi(x_1, ..., x_N) \sim \prod_{j=1}^N \varphi(x_j)$ for large particle numbers. It will almost never be the case that all of the particles are in the right state (e.g. the condensate) but only the overwhelming majority. Therefore, a state like

$$\tilde{\psi} = \prod_{1}^{N-1} \varphi(x_j) \otimes \varphi_{\perp}(x_N)$$

with $\varphi_{\perp} \perp \varphi$ should be considered close to a full product. But the L^2 -norms are quite different:

$$\left\| \prod_{j=1}^{N} \varphi(x_j) - \tilde{\psi} \right\|_{2}^{2} = 1 \cdot \langle \varphi - \varphi_{\perp}, \varphi - \varphi_{\perp} \rangle = 2,$$

independent of the particle number. Instead, we may use closeness of the reduced density matrices in trace norm

$$\left\| \mu^{\psi} - \left| \varphi \right\rangle \left\langle \varphi \right| \right\|_{\mathrm{tr}},$$

or equivalently, smallness of α , as a good notion for closeness. There, the difference between $\tilde{\psi}$ and a full product would be of order $\frac{1}{N}$.