

**PHYSICS 210A : STATISTICAL PHYSICS
FINAL EXAM SOLUTIONS**

(1) Provide clear, accurate, and brief answers for each of the following:

(a) A particle in $d = 3$ dimensions has the dispersion $\varepsilon(\mathbf{k}) = \varepsilon_0 \exp(ka)$. Find the density of states per unit volume $g(\varepsilon)$. Sketch your result. [4 points]

(a) Inverting the dispersion relation, we obtain $k(\varepsilon) = a^{-1} \ln(\varepsilon/\varepsilon_0) \Theta(\varepsilon - \varepsilon_0)$. We then have

$$g(\varepsilon) = \frac{k^2}{2\pi} \frac{dk}{d\varepsilon} = \frac{k^2}{2\pi} \cdot \frac{1}{a\varepsilon_0 e^{ak}}.$$

Thus,

$$g(\varepsilon) = \frac{1}{2\pi^2 a^3} \frac{1}{\varepsilon} \ln^2\left(\frac{\varepsilon}{\varepsilon_0}\right) \Theta(\varepsilon - \varepsilon_0) \quad .$$

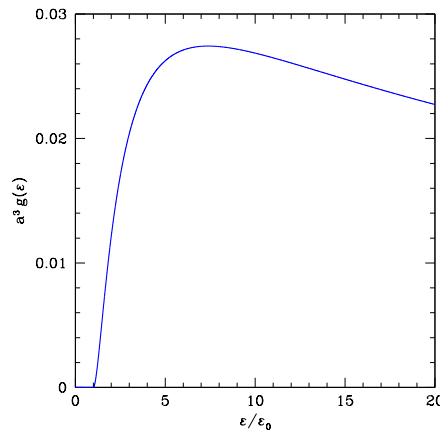


Figure 1: Density of states for problem 1(a).

(b) What is the Maxwell construction? [4 points]

(b) The Maxwell construction is a fix for the van der Waals system and other related phenomenological equations of state $p = p(T, v)$ in which, throughout a region of temperature T , the pressure as a function of volume $p(v)$ is nonmonotonic. This is unphysical since the isothermal compressibility $\kappa_T = -\frac{1}{v} \frac{\partial v}{\partial p}$ becomes negative, which signals an absolute thermal instability, known as *spinodal decomposition*. The regime of instability is even larger than this, however, because of the possibility of *phase separation* into regions of different bulk density. The situation is depicted in Fig. 2. To remedy these defects, one replaces the unstable part of the $p(v)$ curve with a flat line

extending from $v = v_1$ to $v = v_2$ at each temperature T in the unstable region, such that

$$p(T, v_1) = p(T, v_2) = \frac{1}{v_2 - v_1} \int_{v_1}^{v_2} dv p(T, v) \quad .$$

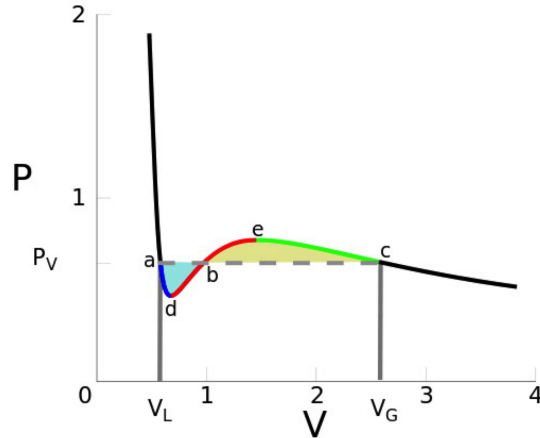


Figure 2: The Maxwell construction corrects a nonmonotonic $p(v)$ to include a flat section, known as the coexistence region, which guarantees that the Helmholtz free energy of the system is at a true minimum. The system is absolutely unstable between volumes v_d and v_e . For $v \in [v_a, v_d]$ or $v \in [v_e, v_c]$, the solution is unstable with respect to phase separation.

(c) For the free energy density $f = \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4$, what does it mean to say that ‘a first order transition preempts the second order transition’? [4 points]

(c) In the absence of a cubic term there is a second order transition at $a = 0$, assuming $b > 0$ for stability. The ordered phase, for $a < 0$, has a spontaneous moment $m \neq 0$. When the cubic term is present, a *first order* (i.e. discontinuous) transition, where m jumps from $\frac{2y}{3b}$, takes place at $a = \frac{2y^2}{9b} > 0$. Thus, as a is decreased from large values, the first order transition takes place before a reaches $a = 0$, hence we say that the second order transition that *would have* occurred at $a = 0$ is *preempted*. Typically we write $a \propto T - T_c^0$, where T_c^0 is what the second order transition temperature would be in the case $y = 0$.

(d) A system of noninteracting bosons has a power law dispersion $\varepsilon(\mathbf{k}) = Ak^\sigma$. What is the condition on the power σ and the dimension d of space such that Bose condensation will occur at some finite temperature? [4 points]

(d) At $T = T_{\text{BEC}}$, we have the relation

$$n = \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\varepsilon(\mathbf{k})/k_B T_{\text{BEC}}} - 1} \quad .$$

If the integral fails to converge, then there is no finite temperature solution and no Bose condensation. For small k , we may expand the exponential in the denominator, and we find the occupancy function behaves as $k_B T_{\text{BEC}}/\varepsilon(\mathbf{k}) \propto k^{-\sigma}$. From the integration metric, in d -dimensional polar coordinates, we have $d^d k = \Omega_d k^{d-1} dk$, where Ω_d is the surface area of the d -dimensional unit sphere. Thus, the integrand is proportional to $k^{d-\sigma-1}$. For convergence, then, we require $d > \sigma$. This is the condition for finite temperature Bose condensation.

- (e) Sketch what the radial distribution function $g(r)$ looks like for a simple fluid like liquid argon. Identify any relevant length scales, as well as the limiting value for $g(r \rightarrow \infty)$. [4 points]

- (e) See Fig. 3. Note that $g(\infty) = 1$, and $g(r) = 0$ for $r < a$, where a is the hard sphere core diameter.

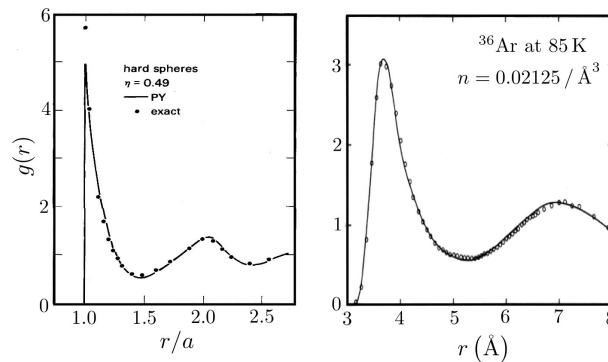


Figure 3: Pair distribution functions for hard spheres of diameter a at volume filling fraction $\eta = \frac{\pi}{6} a^3 n = 0.49$ (left) and for liquid Argon at $T = 85$ K (right).

- (f) ν moles of ideal gaseous argon at an initial temperature T_A and volume $V_A = 1.0$ L undergo an adiabatic free expansion to an intermediate state of volume $V_B = 2.0$ L. After coming to equilibrium, this process is followed by a reversible adiabatic expansion to a final state of volume $V_C = 3.0$ L. Let S_A denote the initial entropy of the gas. Find the temperatures $T_{B,C}$ and the entropies $S_{B,C}$. Then repeat the calculation assuming the first expansion (from A to B) is a reversible adiabatic expansion and the second (from B to C) an adiabatic free expansion. [4 points]
- (f) Argon is a monatomic ideal gas, thus $\gamma = c_p/c_V = \frac{5}{3}$. The adiabatic equation of state is $d(TV^{\gamma-1}) = 0$. The entropy of a monatomic ideal gas is $S = \frac{3}{2} N k_B \ln(E/N) + N k_B \ln(V/N) + Na$ where a is a constant. During an adiabatic free expansion, $\Delta E = Q = W = 0$. We can now construct the following table:
- (g) Explain how the Maxwell-Boltzmann limit results, starting from the expression for $\Omega_{\text{BE/FD}}(T, V, \mu)$. [4 points]

	T_B	T_C	$S_B - S_A$	$S_C - S_A$
AB free / BC reversible	T_A	$(3/2)^{-2/3} T_A$	$\nu R \ln 2$	$\nu R \ln 2$
AB reversible / BC free	$2^{-2/3} T_A$	$2^{-2/3} T_A$	0	$\nu R \ln(3/2)$

(g) We have

$$\Omega_{\text{BE/FD}} = \pm k_B T \sum_{\alpha} \ln(1 \mp z e^{-\varepsilon_{\alpha}/k_B T}) .$$

The MB limit occurs when the product $z e^{-\varepsilon_{\alpha}/k_B T} \ll 1$, in which case

$$\Omega_{\text{BE/FD}} \longrightarrow \Omega_{\text{MB}} = -k_B T \sum_{\alpha} e^{(\mu - \varepsilon_{\alpha})/k_B T} ,$$

where the sum is over all energy eigenstates of the single particle Hamiltonian.

(h) For the one-dimensional spin-1 Ising model $\hat{H} = -J \sum_n S_n S_{n+1}$, where each $S_n \in \{-1, 0, 1\}$, write down the transfer matrix. [4 points]

(h) The transfer matrix is given by

$$R_{SS'} = \exp(\beta J S S') = \begin{pmatrix} \exp(\beta J) & 1 & \exp(-\beta J) \\ 1 & 1 & 1 \\ \exp(-\beta J) & 1 & \exp(\beta J) \end{pmatrix} ,$$

where $\beta = 1/k_B T$.

(2) The density of states per unit volume for a particle in three space dimensions is

$$g(\varepsilon) = \frac{\varepsilon (\varepsilon^2 + \Delta^2)}{\Omega \Delta^4} \Theta(\varepsilon) .$$

(a) What are the dimensions of the constant Ω ? [6 points]

(b) Find the single particle dispersion $\varepsilon(\mathbf{k})$. [7 points]

(c) Assuming the particles obey photon statistics find their density $n(T)$. [7 points]

(d) Assuming the particles are bosons, find the Bose condensation temperature $T_c(n)$. [7 points]

(e) Assuming the particles are fermions, find the Fermi energy $\varepsilon_F(n)$. [7 points]

Solution :

(a) $[\Omega] = V$ (i.e. volume).

(b) We have

$$g(\varepsilon) d\varepsilon = \frac{d^3k}{(2\pi)^3} = \frac{k^2}{2\pi^2} \frac{dk}{d\varepsilon} \quad \Rightarrow \quad d\left(\frac{k^3}{6\pi^2}\right) = d\left(\frac{\frac{1}{4}\varepsilon^4 + \frac{1}{2}\Delta^2\varepsilon^2}{\Omega\Delta^4}\right).$$

Note that Ω has units of volume. Integrating, we have

$$\frac{1}{4}\varepsilon^4 + \frac{1}{2}\Delta^2\varepsilon^2 - \frac{\Delta^4\Omega k^3}{6\pi^2} = 0,$$

with solution

$$\varepsilon(k) = \Delta \sqrt{\left[1 + \left(\frac{2\Omega k^3}{3\pi^2}\right)\right]^{1/2} - 1}.$$

In the limit $k \rightarrow 0$, one finds $\varepsilon(k) = \Delta \left(\frac{\Omega}{3\pi^2}\right)^{1/2} k^{3/2}$.

(c) The photon density is

$$\begin{aligned} n &= \int_0^\infty d\varepsilon \frac{g(\varepsilon)}{e^{\varepsilon/k_B T} - 1} = \frac{1}{\Omega} \int_0^\infty dx \frac{1}{e^x - 1} \left\{ \left(\frac{k_B T}{\Delta}\right)^4 x^3 + \left(\frac{k_B T}{\Delta}\right)^2 x \right\} \\ &= \frac{\Gamma(4)\zeta(4)}{\Omega} \left(\frac{k_B T}{\Delta}\right)^4 + \frac{\Gamma(2)\zeta(2)}{\Omega} \left(\frac{k_B T}{\Delta}\right)^2, \end{aligned}$$

since

$$\int_0^\infty dx \frac{x^{p-1}}{e^x - 1} = \Gamma(p) \zeta(p).$$

Now $\Gamma(4) = 6$, $\Gamma(2) = 1$, $\zeta(4) = \frac{\pi^4}{90}$, and $\zeta(2) = \frac{\pi^2}{6}$, so

$$n(T) = \frac{1}{15\Omega} \left(\frac{\pi k_B T}{\Delta}\right)^4 + \frac{1}{6\Omega} \left(\frac{\pi k_B T}{\Delta}\right)^2.$$

(d) The equation for T_c is $n(T_c) = n$, where $n(T_c)$ is the photon statistics (i.e. $\mu = 0$) density at $T = T_c$. Solving the above quadratic equation in T^2 , we find

$$k_B T_c = \sqrt{\frac{5}{4}} \frac{\Delta}{\pi} \sqrt{\left[1 + \frac{48}{5} n\Omega\right]^{1/2} - 1}.$$

(e) We have, for fermions at $T = 0$,

$$n = \int_0^{\varepsilon_F} d\varepsilon g(\varepsilon) = \frac{\frac{1}{4}\varepsilon_F^4 + \frac{1}{2}\Delta^2\varepsilon_F^2}{\Omega\Delta^4},$$

and hence

$$\varepsilon_F(n) = \Delta \sqrt{[1 + 4n\Omega]^{1/2} - 1} .$$

(3) Consider the three-state (\mathbb{Z}_3) clock model, with Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \hat{n}_i \cdot \hat{n}_j ,$$

where the interaction is between all unit vectors \hat{n}_i and \hat{n}_j lying on neighboring sites on a regular lattice of coordination number z . Each \hat{n}_i can take one of three possible values $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$, where

$$\hat{e}_1 = \hat{x} \quad , \quad \hat{e}_2 = -\frac{1}{2} \hat{x} + \frac{\sqrt{3}}{2} \hat{y} \quad , \quad \hat{e}_3 = -\frac{1}{2} \hat{x} - \frac{\sqrt{3}}{2} \hat{y} \quad .$$

In service of analyzing this model, consider the variational density matrix $\varrho_N(\hat{n}_1, \dots, \hat{n}_N) = \prod_i \varrho_1(\hat{n}_i)$, where the single site variational density matrix is

$$\varrho_1(\hat{n}) = \frac{1 + 2u}{3} \delta_{\hat{n}, \hat{e}_1} + \frac{1 - u}{3} \delta_{\hat{n}, \hat{e}_2} + \frac{1 - u}{3} \delta_{\hat{n}, \hat{e}_3} \quad ,$$

where u is the variational parameter.

- What is the allowed range for u ? Show that the density matrix is appropriately normalized. [4 points]
- Find the variational energy $E(u) = \text{Tr}(\varrho_N H)$. [6 points]
- Find the entropy $S(u) = -k_B \text{Tr}(\varrho_N \ln \varrho_N)$. [6 points]
- Adimensionalize by defining $f = F/NzJ$ and $\theta = k_B T/zJ$ and find the dimensionless free energy density $f(u, \theta)$. Do you expect a first or second order transition? Why? [6 points]
- Find the self-consistent mean field equation for u . [6 points]
- Analyze the model keeping only terms up to order u^4 in $f(u, \theta)$. Find the location of the phase transition and remark on whether it is first or second order. [6 points]

The following low order Taylor expansion may prove useful:

$$(1 + \varepsilon) \ln(1 + \varepsilon) = \varepsilon + \frac{1}{2} \varepsilon^2 - \frac{1}{6} \varepsilon^3 + \frac{1}{12} \varepsilon^4 + \mathcal{O}(\varepsilon^5) \quad .$$

Solution :

(a) Since $\varrho_1(\hat{n})$ is the probability that a site is in state \hat{n} , and since probabilities are constrained to lie on the interval $[0, 1]$, we must have $u \in [-\frac{1}{2}, 1]$. Clearly we have $\text{Tr} \varrho_1(\hat{n}) = \sum_{j=1}^3 \varrho_1(\hat{e}_j) = 1$, which is the appropriate normalization.

(b) For any nearest neighbor pair $\langle ij \rangle$, the energy is $-J$ if $\hat{n}_i = \hat{n}_j$ and $+\frac{1}{2}J$ if $\hat{n}_i \neq \hat{n}_j$ (since $\hat{e}_1 \cdot \hat{e}_2 = \hat{e}_1 \cdot \hat{e}_3 = \hat{e}_2 \cdot \hat{e}_3 = -\frac{1}{2}$). Remembering that there are $\frac{1}{2}Nz$ nearest neighbor links, where N is the number of sites,

$$\begin{aligned} E &= \text{Tr}(\varrho_N H) = \frac{1}{2}Nz \text{Tr}_{\hat{n}_i} \text{Tr}_{\hat{n}_j} \left(\varrho_1(\hat{n}_i) \varrho_1(\hat{n}_j) (-J\hat{n}_i \cdot \hat{n}_j) \right) \\ &= \frac{1}{2}Nz \left\{ \left(\frac{1+2u}{3} \right)^2 \cdot (-J) + 2 \left(\frac{1-u}{3} \right)^2 \cdot (-J) + 4 \left(\frac{1+2u}{3} \right) \left(\frac{1-u}{3} \right) \cdot \left(\frac{1}{2}J \right) + 2 \left(\frac{1-u}{3} \right)^2 \cdot \left(\frac{1}{2}J \right) \right\} \\ &= -\frac{1}{2}NzJu^2 \quad . \end{aligned}$$

Note among two spins, with nine possible configurations, three have energy $E_{ij} = -J$: one with $\hat{n}_i = \hat{n}_j = \hat{e}_1$ with probability $\left(\frac{1+2u}{3}\right)^2$, and two with $\hat{n}_i = \hat{n}_j = \hat{e}_{2,3}$, each with probability $\left(\frac{1-u}{3}\right)^2$. The remaining six configurations all have energy $E_{ij} = +\frac{1}{2}J$. In four of these, one from \hat{n}_i and \hat{n}_j is equal to \hat{e}_1 , and the other is either \hat{e}_2 or \hat{e}_3 . Each occurs with probability $\left(\frac{1+2u}{3}\right)\left(\frac{1-u}{3}\right)$. In the remaining two cases, $\hat{n}_i = \hat{e}_2$ and $\hat{n}_j = \hat{e}_3$, or $\hat{n}_i = \hat{e}_3$ and $\hat{n}_j = \hat{e}_2$, each with probability $\left(\frac{1-u}{3}\right)^2$.

An easier way to get this result is to compute

$$\text{Tr}(\hat{n} \varrho_1(\hat{n})) = \left(\frac{1+2u}{3} \right) \hat{e}_1 + \left(\frac{1-u}{3} \right) (\hat{e}_2 + \hat{e}_3) = u \hat{x} \quad ,$$

and thus $E = -\frac{1}{2}NzJ \langle \hat{n} \rangle^2 = -\frac{1}{2}NzJu^2$.

(c) The entropy is $S = -k_B \text{Tr}(\varrho_N \ln \varrho_N) = -Nk_B \text{Tr}(\varrho_1 \ln \varrho_1) = Ns$, with

$$s(u) = -k_B \text{Tr}(\varrho_1 \ln \varrho_1) = -\ln 3 + \frac{1}{3}(1+2u) \ln(1+2u) + \frac{2}{3}(1-u) \ln(1-u) \quad .$$

(d) Doing the usual thang,

$$\begin{aligned} f(u, \theta) &= -\frac{1}{2}u^2 + \theta s(u) \\ &= -\frac{1}{2}u^2 + \frac{1}{3}\theta(1+2u) \ln(1+2u) + \frac{2}{3}\theta(1-u) \ln(1-u) \quad . \end{aligned}$$

Since $f(u) \neq f(-u)$, there is no \mathbb{Z}_2 symmetry, and we should expect a cubic term in the resulting Landau free energy expansion, suggesting a first order transition will preempt any second order transition in this model.

(e) The mean field equation is obtained by setting $\partial f / \partial u = 0$. Thus,

$$u = \frac{2}{3} \theta \ln \left(\frac{1+2u}{1-u} \right) \quad .$$

(f) Expanding $f(u, \theta)$ to fourth order in the order parameter u , we obtain

$$f(u, \theta) = \left(\theta - \frac{1}{2} \right) u^2 - \frac{1}{3} \theta u^3 + \frac{1}{2} \theta u^4 + \mathcal{O}(u^5) \quad .$$

As predicted, there is a cubic term, hence the second order transition which would have occurred at $\theta = \frac{1}{2}$ is preempted by a first order transition. For a quartic Landau free energy $f = \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4$, the first order transition sets in at $a = 2y^2/9b$. We have $a = 2\theta - 1$, $y = \theta$, and $b = 2\theta$, resulting in $\theta_c = \frac{9}{17} > \frac{1}{2}$. The value of u just above the transition is $u_c = 3a_c/y = 2y/3b = \frac{1}{3}$.

Note that this result is only valid for the quartic Landau theory, and that to find the location of the first order transition in the original model, we must simultaneously solve the mean field equation $f'(u) = 0$ and the condition $f(u) = f(0)$. This gives two conditions on the two unknowns (u, θ) at the first order transition. If we define the function

$$\psi(u) = \ln 3 - s(u) = \frac{1}{3}(1+2u)\ln(1+2u) + \frac{2}{3}(1-u)\ln(1-u) \quad ,$$

then $f(u) = -\frac{1}{2}u^2 + \theta\psi(u)$ and the mean field equation is $u = \theta\psi'(u)$. Note that $\psi(0) = 0$. Next, we set $f(u) = f(0) = 0$ to find when the local minimum at nonzero u crosses the axis and becomes a global minimum. Eliminating θ results in the equation

$$\psi(u) = \frac{1}{2}u\psi'(u) \quad .$$

After obtaining the solution for u_c , we substitute into the mean field equation to obtain $\theta_c = u_c/\psi'(u_c)$. For our model, the solution can be found exactly! It occurs for

$$u_c = \frac{1}{2} \quad , \quad \theta_c = \frac{3}{8\ln 2} = 0.54101 \quad .$$

Thus the exact value of θ_c lies above $\theta = \frac{1}{2}$, where the coefficient of the quadratic term in the Landau expansion changes sign, and above the value $\theta_c^{\text{TL}} = \frac{9}{17} = 0.5294$ from the truncated Landau expansion in which terms beyond $\mathcal{O}(u^4)$ were dropped.

Indeed, consider a generalized version of our model where $e(u) = E/NJz = -\kappa u^2$ and

$$s(u) = -\left(\frac{1+(p-1)u}{p}\right)\ln\left(\frac{1+(p-1)u}{p}\right) - (p-1)\left(\frac{1-u}{p}\right)\ln\left(\frac{1-u}{p}\right) \quad .$$

In the problem studied here, $\kappa = \frac{1}{2}$ and $p = 3$. From $f(u) = e(u) - \theta s(u)$ and $f'(u) = 0$ one derives the mean field equation

$$u = \theta\left(\frac{p-1}{2\kappa p}\right)\ln\left(\frac{1+(p-1)u}{1-u}\right) \quad .$$

The exact solution for (u, θ) to the simultaneous equations $f(u) = f(0)$ and $f'(u) = 0$ is found to be at

$$u_c = \frac{p-2}{p-1} \quad , \quad \theta_c = \frac{p(p-2)\kappa}{(p-1)^2\ln(p-1)} \quad .$$

The Landau expansion is found to be

$$f(u) = -\theta\ln p + \frac{1}{2}au^2 - \frac{1}{3}yu + \frac{1}{4}bu^4 + \mathcal{O}(u^5)$$

where

$$a = (p-1)\theta - 2\kappa \quad , \quad y = \frac{1}{2}(p-1)(p-2)\theta \quad , \quad b = \frac{1}{3}(p-1)(p^2 - 3p + 3)\theta \quad .$$

If we truncate at fourth order, we find a first order transition at

$$u_c^{\text{TL}} = \frac{p-2}{p^2-3p+3} \quad , \quad \theta_c^{\text{TL}} = \frac{12\kappa}{p-1} \cdot \frac{p^2-3p+3}{5p^2-14p+14} \quad .$$

(4) Write a well-defined expression for the greatest possible number expressible using only five symbols. *Examples:* $1 + 2 + 3$, 10^{100} , $\Gamma(99)$. [50 quatloos extra credit]

Solution :

Using conventional notation, my best shot would be $9^{9^{9^9}}$. This is a very big number indeed: $9^9 \approx 3.73 \times 10^8$, so $9^{9^9} \sim 10^{3.7 \times 10^8}$, and $9^{9^{9^9}} \sim 10^{10^{10^{3.7 \times 10^8}}}$. But in the world of big numbers, this is still tiny. For a fun diversion, use teh google to learn about the Ackermann sequence and Knuth's up-arrow notation. Using Knuth's notation, described in

http://en.wikipedia.org/wiki/Knuth's_up-arrow_notation ,

one could write $9 \uparrow^{99} 9$, which is vastly larger than the puny $9^{9^{9^9}}$. But even *these* numbers are modest compared with something called the "Busy Beaver sequence", which is a concept from computer science and Turing machines. For a very engaging essay on large numbers, see <https://www.scottaaronson.com/blog/?p=3445>.