

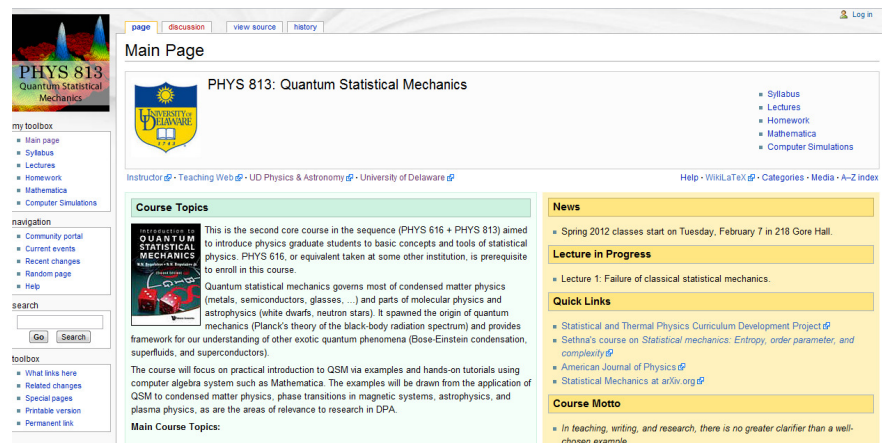
Lecture 1: Failure of Classical Statistical Mechanics

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PHYS 813: Quantum Statistical Mechanics

<http://wiki.physics.udel.edu/phys813>

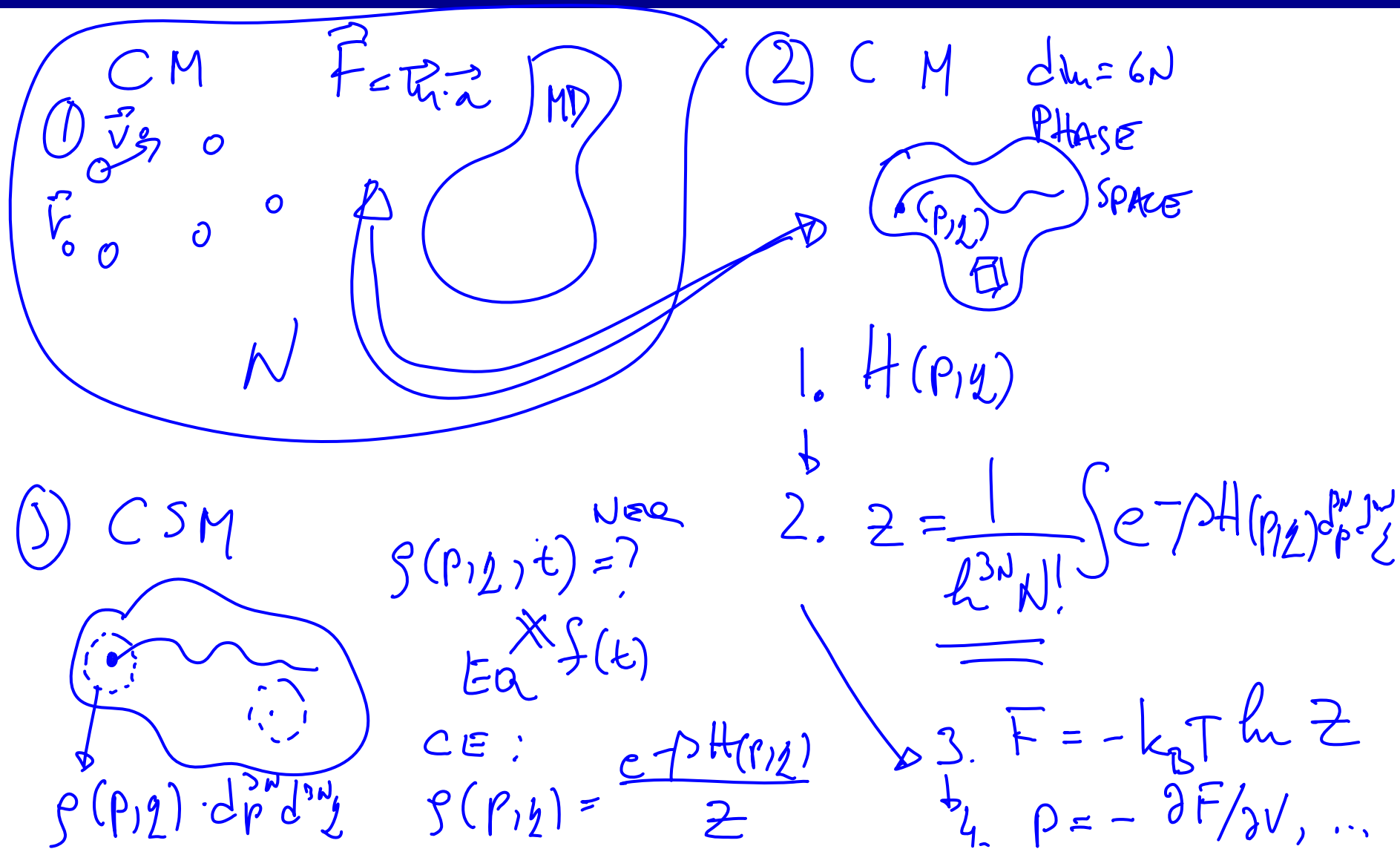


The screenshot shows the main page of the PHYS 813 Wiki. The page title is "PHYS 813: Quantum Statistical Mechanics". The content includes a "Course Topics" section with a description of the course as the second core course in the sequence (PHYS 616 + PHYS 813) aimed at introducing physics graduate students to basic concepts and tools of statistical physics. It also mentions that quantum statistical mechanics governs most of condensed matter physics (metals, semiconductors, glasses, ...) and parts of molecular physics and astrophysics (white dwarfs, neutron stars). The page also features a "News" section with a link to the Spring 2012 classes, a "Lecture in Progress" section for Lecture 1, and a "Quick Links" section with links to the syllabus, lectures, homework, mathematics, and computer simulations. A "Course Motto" is also present at the bottom.

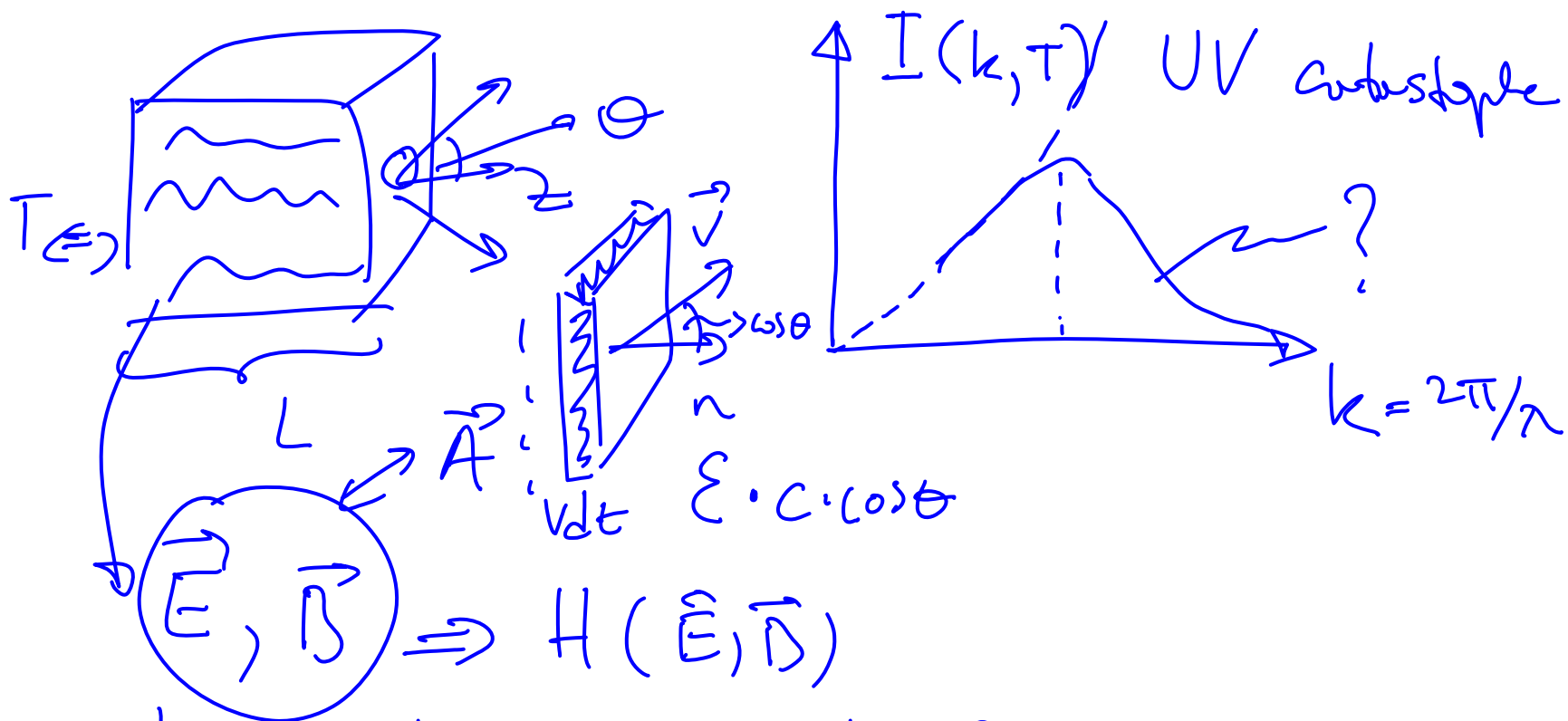
PHYS 813: Quantum statistical mechanics

Failure of classical statistical mechanics

The Algorithm of Classical Statistical Mechanics for Canonical Ensemble



Electromagnetic Field in Cavity at Temperature T



$$W_{EM} = W_E + W_B = \frac{1}{2} \epsilon \int_{\text{cube}} E^2 dV + \frac{1}{2\mu_0} \int_{\text{cube}} B^2 dV$$

$$\vec{E} = -\frac{\partial \vec{A}}{\partial t}, \quad \vec{B} = \nabla \times \vec{A}; \quad \vec{A} = A(x, y, z, t) = A(x, y+L, z, t) = \dots$$

Decomposition of EM Field into Normal Modes

$$\vec{A}(\vec{r}, t) = \sum_{\vec{k}, \alpha} \left(a_{\vec{k}, \alpha} e^{i\vec{k}\cdot\vec{r}} + a_{\vec{k}, \alpha}^* e^{-i\vec{k}\cdot\vec{r}} \right)$$

$$\nabla \cdot \vec{E} = 0 \Rightarrow \vec{k} \cdot \vec{E} = 0, \quad \alpha = 1, 2$$

$$W_{EM} = \frac{1}{2} \sum_{\vec{k}, \alpha} \left(|P_{\vec{k}, \alpha}|^2 + \omega_{\alpha}(\vec{k}) |Q_{\vec{k}, \alpha}|^2 \right) \quad \text{mod } (a_{\vec{k}, \alpha} + a_{-\vec{k}, \alpha}^*)$$

$$\hookrightarrow \alpha i \omega_{\alpha}(\vec{k}) \cdot (a_{\vec{k}, \alpha} - a_{-\vec{k}, \alpha}^*)$$

$$\omega_{\alpha}(\vec{k}) = c \cdot |\vec{k}| = c \cdot k, \quad \alpha = 1, 2$$

$$\vec{k}_{\alpha} \rightarrow k_{\alpha} T \quad \vec{k} = \frac{2\pi}{L} (n_x, n_y, n_z)$$

Quantization of Normal Modes and Canonical Partition Function

$$H^{QM} = \sum_{\vec{k}, \alpha} \hbar \omega_{\alpha}(\vec{k}) \left(n_{\alpha}(\vec{k}) + \frac{1}{2} \right)$$

$\mathcal{L} H_0$

$$Z \stackrel{\text{PHYS 616}}{=} \sum_{\vec{k}} e^{-\beta E_{\vec{k}}}$$

$$\text{PHYS 616} \rightarrow Z = Z_1^N$$

$$\sum_{\{n_{\alpha}(\vec{k})\}} e^{-\beta H^{QM}} = \prod_{\vec{k}, \alpha} \left[\sum_{n_{\alpha}(\vec{k})=0}^{\infty} e^{-\beta \hbar \omega_{\alpha}(\vec{k}) (n_{\alpha}(\vec{k}) + 1/2)} \right]$$

$$= \prod_{\vec{k}, \alpha} \frac{e^{-\beta \hbar \omega_{\alpha}(\vec{k}) / 2}}{1 - e^{-\beta \hbar \omega_{\alpha}(\vec{k})}}$$

Evaluation of Canonical Partition Function and Thermodynamic Quantities

$$F = -k_B T \ln Z,$$

$$p = -\partial F / \partial V = \left(p_0 \right) + \frac{1}{V} \bar{\epsilon}$$

$$p_0 \left| p_0' \right| p_0$$

$$E = -\frac{\partial}{\partial \beta} \ln Z$$

$$-\ln Z = \sum_{\vec{k}, \alpha} \left(\frac{\beta \epsilon_{\vec{k}, \alpha}}{2} + \ln(1 - e^{-\beta \epsilon_{\vec{k}, \alpha}}) \right)$$

$$\bar{\epsilon} = -\frac{\partial}{\partial \beta} \ln Z = E_0 \cdot V + \sum_{\vec{k}, \alpha} \frac{e^{-\beta \epsilon_{\vec{k}, \alpha}}}{1 - e^{-\beta \epsilon_{\vec{k}, \alpha}}} \cdot \epsilon_{\vec{k}, \alpha} = E_0 V + \sum_{\vec{k}, \alpha} \frac{\epsilon_{\vec{k}, \alpha}}{e^{\beta \epsilon_{\vec{k}, \alpha}} - 1}$$

$$\sum_{\vec{k}, \alpha} f(\vec{k}) \rightarrow \frac{1}{\Delta \vec{k}} \sum_{\vec{k}, \alpha} f(\vec{k}) \Delta \vec{k} \xrightarrow{\Delta \vec{k} \rightarrow 0} \frac{V}{(2\pi)^3} \int f(\vec{k}) d^3 \vec{k}$$

Total Energy Flux Emitted by Cavity and Stefan-Boltzmann Law

$$E^* = 2 \frac{V}{(2\pi)^3} \int \frac{\hbar c k}{e^{\beta \hbar c k} - 1} d^3k = 2 \frac{V}{(2\pi)^3} \int \frac{\hbar c k}{e^{\beta \hbar c k} - 1} \hbar^2 \sin\theta d\theta d\phi$$

$$x = \beta \hbar c k, \quad E^*/V = \frac{\hbar c}{\pi^2} \left(\frac{\hbar^3 T}{\hbar c} \right)^3 \int_0^\infty \frac{dx x^3}{e^x - 1} \quad \pi^4/15$$

$$= \frac{\pi^2}{15} \left(\frac{\hbar^4 T}{\hbar c} \right)^3 \hbar^3 T$$

$$\Phi = \frac{E^*}{V} \cdot \langle C_\perp \rangle \quad \pi/2 \rightarrow \left(\frac{\pi^2 \hbar^4 T^4}{60 \hbar^3 c^2} \right) \text{ Stefan-Boltzmann law}$$

$$\langle C_\perp \rangle = \frac{c}{4\pi} \int_0^\pi \cos\theta \, 2\pi \sin\theta \, d\theta = c/4$$

Energy Flux Emitted by Cavity at Each Wavevector (or Wavelength)

$$\frac{E^*(T)}{V} = \int dk \Sigma(k, T)$$

$$I(k, T) dk \rightarrow [k, k+dk]$$

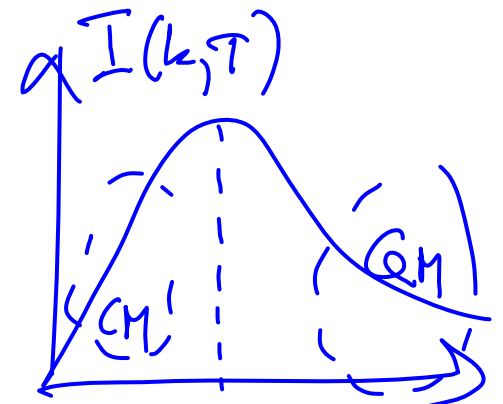
$$k^* \approx \frac{k_B T}{hc}$$

$$\Sigma(k, T) \cdot \frac{c}{4} = I(k, T)$$

$$\Sigma(k, T) = \frac{kc}{\pi^2} \cdot \frac{k^3}{e^{ptck} - 1}$$

$$I(k, T) = \frac{c}{4}$$

$$k \ll k^* \Rightarrow I(k, T) = \frac{c k_B T k^2}{4\pi^2}; \quad k \gg k^*, \quad I(k, T) = \frac{hc^2 k^3}{4\pi^2} e^{-\frac{ptck}{k_B T}}$$



$$k^*(T) \approx \frac{k_B T}{hc}$$