COHERENCE DOMAINS in MATTER INTERACTING with RADIATION

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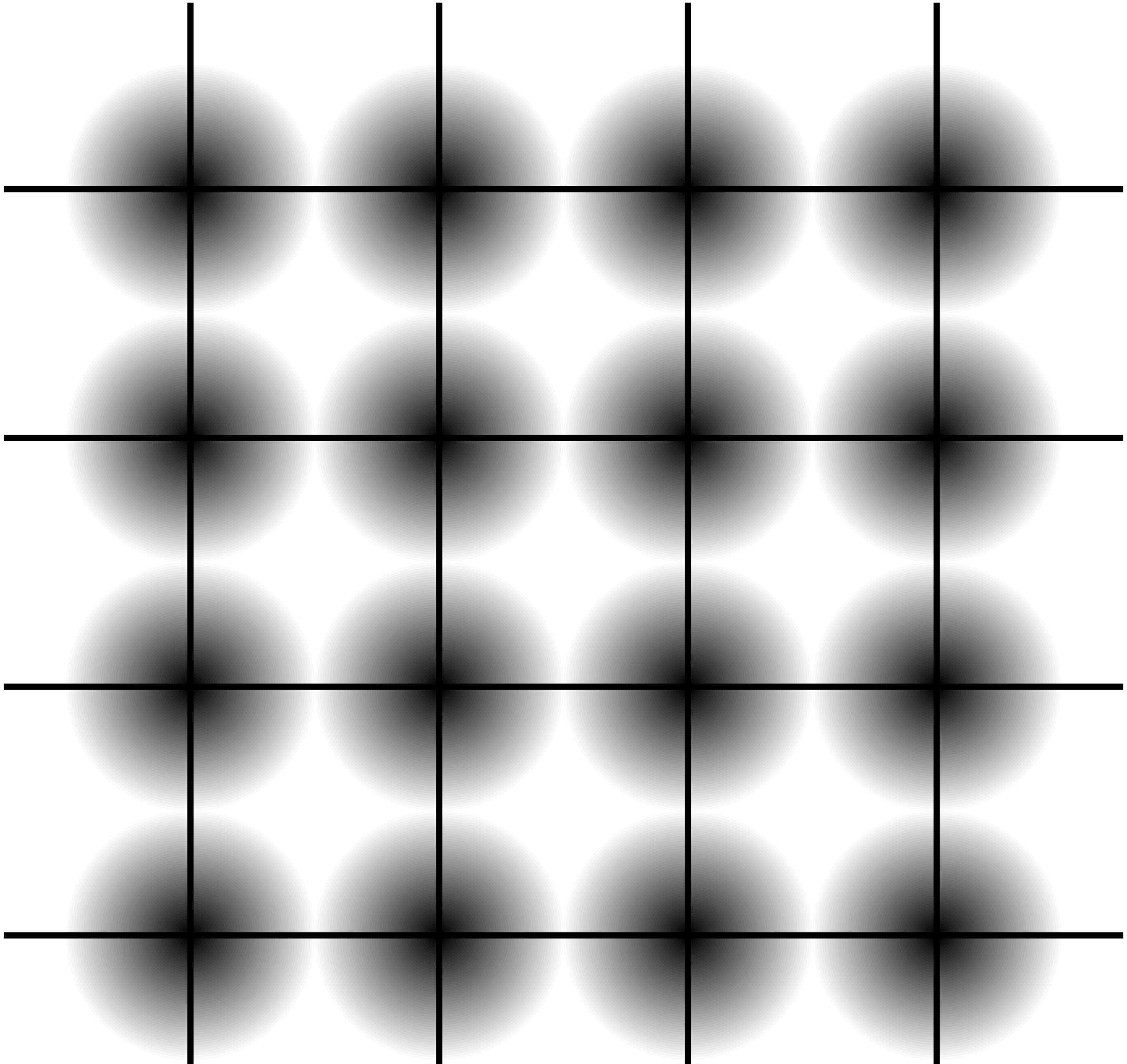

2

1) Imagine a piece of matter, either gas, liquid or solid

2) Imagine a series of excitation levels, atomic, molecular

3) Imagine the interaction of this substance with the EM radiation (dipolar int)

Now, you are ready to hearing me telling you something SURPRISING!

Electromagnetic Field

Vector potential

$$\mathbf{A}(\mathbf{r}) = \sum_{\alpha\mathbf{k}} \sqrt{\frac{2\pi\hbar c^2}{V\omega_k}} \left[\mathbf{e}_\alpha(\mathbf{k}) a_{\alpha\mathbf{k}} e^{i\mathbf{kr}} + \mathbf{e}^*_\alpha(\mathbf{k}) a^*_{\alpha\mathbf{k}} e^{-i\mathbf{kr}}\right]$$

The fields: $\mathbf{E} = -(1/c)\partial\mathbf{A}/\partial t$, $\mathbf{H} = curl\mathbf{A}$

Three Maxwell's eqs: $curl\mathbf{E} = -\frac{1}{c}\partial\mathbf{H}/\partial t$, $div\mathbf{H} = 0$, $div\mathbf{E} = 0$

The free Lagrangian:

$$L_f = \frac{1}{8\pi}\int d\mathbf{r}\left(E^2 - H^2\right) =$$

$$= \sum_{\alpha\mathbf{k}} \frac{\hbar}{4\omega_k}\left(\dot{a}_{\alpha\mathbf{k}}\dot{a}_{-\alpha-\mathbf{k}} + \dot{a}^*_{\alpha\mathbf{k}}\dot{a}^*_{-\alpha-\mathbf{k}} + \dot{a}_{\alpha\mathbf{k}}\dot{a}^*_{\alpha\mathbf{k}} + \dot{a}^*_{\alpha\mathbf{k}}\dot{a}_{\alpha\mathbf{k}}\right) -$$

$$- \sum_{\alpha\mathbf{k}} \frac{\hbar\omega_k}{4}\left(a_{\alpha\mathbf{k}}a_{-\alpha-\mathbf{k}} + a^*_{\alpha\mathbf{k}}a^*_{-\alpha-\mathbf{k}} + a_{\alpha\mathbf{k}}a^*_{\alpha\mathbf{k}} + a^*_{\alpha\mathbf{k}}a_{\alpha\mathbf{k}}\right)$$

The interacting Lagrangian:

$$L_{int} = \frac{1}{c}\int d\mathbf{r}\cdot\mathbf{jA} = \sum_{\alpha\mathbf{k}}\sqrt{\frac{2\pi\hbar}{\omega_k}}\left[\mathbf{e}_\alpha(\mathbf{k})\mathbf{j}^*(\mathbf{k})a_{\alpha\mathbf{k}} + \mathbf{e}^*_\alpha(\mathbf{k})\mathbf{j}(\mathbf{k})a^*_{\alpha\mathbf{k}}\right]$$

Eq of motion:

$$\ddot{a}_{\alpha\mathbf{k}} + \ddot{a}^*_{-\alpha-\mathbf{k}} + \omega_k^2 \left(a_{\alpha\mathbf{k}} + a^*_{-\alpha-\mathbf{k}} \right) = \sqrt{\frac{8\pi\omega_k}{\hbar}} \mathbf{e}^*_\alpha(\mathbf{k})\mathbf{j}(\mathbf{k})$$

The fourth Maxwell's eq:

$$curl\mathbf{H} = (1/c)\partial\mathbf{E}/\partial t + 4\pi\mathbf{j}/c$$

Matter Field (Substance)

Atoms, molecules $i = 1, 2...N$ (non-interacting)

$$H_s = \sum_i H_s(i)$$

Wavefunctions:

$$H_s(i)\varphi_n(j) = \varepsilon_n \delta_{ij} \ , \ \int d\mathbf{r} \varphi_n^*(i)\varphi_m(j) = \delta_{ij}\delta_{nm}$$

The field:

$$\psi_n = \sum_i c_{ni} \varphi_n(i) \ , \ H_s \psi_n = \varepsilon_n \psi_n$$

$$\sum_i |c_{ni}|^2 = 1 \ , \ \psi_n = \frac{1}{\sqrt{N}} \sum_i e^{i\theta_{ni}} \varphi_n(i)$$

The quantization of the field:

$$\Psi = \sum_n b_n \psi_n$$

Boson operators: $N \to \infty$ (any occupancy)

$$N = \sum_n b_n^* b_n$$

The Lagrangian:

$$L_s = \frac{1}{2} \int d\mathbf{r} \left(\Psi^* \cdot i\hbar \partial \Psi / \partial t - i\hbar \partial \Psi^* / \partial t \cdot \Psi \right) - \int d\mathbf{r} \Psi^* H_s \Psi$$

$$L_s = \frac{1}{2} \sum_n i\hbar \left[b_n^* \dot{b}_n - \dot{b}_n^* b_n \right] - \sum_n \varepsilon_n b_n^* b_n$$

Schroedinger's equation:

$$H_s = \sum_n \varepsilon_n b_n^* b_n \ , \ \ i\hbar \dot{b}_n = \varepsilon_n b_n$$

The current density:

$$\mathbf{j}(\mathbf{r}) = \sum_i \mathbf{J}(i)\delta(\mathbf{r} - \mathbf{r}_i) = \frac{1}{V}\sum_{i\mathbf{k}} \mathbf{J}(i) e^{-i\mathbf{k}\mathbf{r}_i} e^{i\mathbf{k}\mathbf{r}} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \mathbf{j}(\mathbf{k}) e^{i\mathbf{k}\mathbf{r}}$$

Remember the interaction with the EM field:

$$L_{int} = \sum_{nm\alpha\mathbf{k}} \sqrt{\frac{2\pi\hbar}{V\omega_k}} \left[\mathbf{e}_\alpha(\mathbf{k})\mathbf{I}^*_{mn}(\mathbf{k}) a_{\alpha\mathbf{k}} + \mathbf{e}^*_\alpha(\mathbf{k})\mathbf{I}_{nm}(\mathbf{k}) a^*_{\alpha\mathbf{k}}\right] b_n^* b_m$$

Note this matrix:

$$\mathbf{I}_{nm}(\mathbf{k}) = \frac{1}{N}\sum_i \mathbf{J}_{nm}(i) e^{-i(\theta_{ni}-\theta_{mi})} e^{-i\mathbf{k}\mathbf{r}_i}$$

Schroedinger's equation again, with interaction:

$$i\hbar\dot{b}_n = \varepsilon_n b_n - \sum_{m\alpha\mathbf{k}} \sqrt{\frac{2\pi\hbar}{V\omega_k}} \left[\mathbf{e}_\alpha(\mathbf{k})\mathbf{I}^*_{mn}(\mathbf{k}) a_{\alpha\mathbf{k}} + \mathbf{e}^*_\alpha(\mathbf{k})\mathbf{I}_{nm}(\mathbf{k}) a^*_{\alpha\mathbf{k}}\right] b_m$$

And Maxwell's equation:

$$\ddot{a}_{\alpha\mathbf{k}} + \ddot{a}^*_{-\alpha-\mathbf{k}} + \omega_k^2 \left(a_{\alpha\mathbf{k}} + a^*_{-\alpha-\mathbf{k}} \right) = \sum_{nm} \sqrt{\frac{8\pi\omega_k}{V\hbar}} \mathbf{e}^*_\alpha(\mathbf{k}) \mathbf{I}_{nm}(\mathbf{k}) b_n^* b_m$$

The most common from of the interacting hamiltonian (Quantum Electrodynamics):

$$H_{int} = -\sum_{nm\alpha\mathbf{k}} \sqrt{\frac{2\pi\hbar}{V\omega_k}} [\mathbf{e}_\alpha(\mathbf{k}) \mathbf{I}^*_{mn}(\mathbf{k}) a_{\alpha\mathbf{k}} e^{\frac{i}{\hbar}(\varepsilon_n - \varepsilon_m - \hbar\omega_k)} +$$

$$+ \mathbf{e}^*_\alpha(\mathbf{k}) \mathbf{I}_{nm}(\mathbf{k}) a^*_{\alpha\mathbf{k}} e^{\frac{i}{\hbar}(\varepsilon_n - \varepsilon_m + \hbar\omega_k)}] b_n^* b_m$$

Coherence Domains

$$L_{int} = \sum_{nm\alpha\mathbf{k}} \sqrt{\frac{2\pi\hbar}{V\omega_k}} F_{nm}(\alpha\mathbf{k}) \left(a_{\alpha\mathbf{k}} + a^*_{-\alpha-\mathbf{k}} \right) b^*_n b_m$$

$$F_{nm}(\alpha\mathbf{k}) = \frac{1}{N} \sum_i \mathbf{e}_\alpha(\mathbf{k}) \mathbf{J}_{nm}(i) e^{i\mathbf{k}\mathbf{r}_i - i(\theta_{ni} - \theta_{mi})}$$

What I want? A classical dynamics!

Note the RANDOM PHASE $i\mathbf{k}\mathbf{r}_i - i\,(\theta_{ni} - \theta_{mi})$! Vanishing interaction!

We may arrange, perhaps, for some $\mathbf{k}$'s, but no thermodynamics!

Way out: A LATTICE!

For any pair (nm) of energy levels: $\mathbf{r}_i = \mathbf{R}_p + \mathbf{r}_{pi}$, spatial lattice $\mathbf{R}_p$, $\mathbf{r}_{pi}$ restricted to the first Wigner-Seitz cell

$\mathbf{R}_p$ such that the magnitudes of its shortest reciprocal vectors $\mathbf{k}_r$, $r = 1, 2, 3$, are equal with the magnitude of the relevant wavevectors $\mathbf{k}$, *i.e.* those wavevectors which satisfy $\hbar\omega_k = \varepsilon_n - \varepsilon_m > 0$; and $\mathbf{k}_r \mathbf{R}_p = 2\pi \times integer$

Only a cubic and a trigonal (rhombohedral) symmetry is thus allowed

A cubic lattice: a periodicity length $\lambda = 2\pi/k$, where k is the magnitude of the relevant wavevector

Again

$$F_{nm}(\alpha\mathbf{k}_r) = \frac{1}{N}\sum_{pi} \mathbf{e}_\alpha(\mathbf{k}_r)\mathbf{J}_{nm}(i)e^{i\mathbf{k}_r\mathbf{r}_{pi} - i(\theta_{ni} - \theta_{mi})}$$

Coherence condition:

$$\mathbf{k}_r\mathbf{r}_{pi} - (\theta_{ni} - \theta_{mi}) = K$$

The subsets $N_{nm}(\alpha\mathbf{k}_r)$: $\mathbf{e}_\alpha(\mathbf{k}_r)\mathbf{J}_{nm}(i) = J_{nm}$

$$F_{nm}(\alpha\mathbf{k}_r) = J_{nm}N_{nm}(\alpha\mathbf{k}_r)/N$$

$$\sum_{(nm)\alpha\mathbf{k}_r} N_{nm}(\alpha\mathbf{k}_r) = N$$

The phase of the internal motion of the i-th particle is correlated to the position of that particle

Long-range order, a cooperative phenomenon

The phase of the internal motion "feels" the particle position

Various pairs (nm): a superposition of such lattices of coherence domains

These lattices can also be one- or two-dimensional

A one-dimensional lattice of coherence domains: a set of parallel sheets (layered structure), with the relevant periodicity length λ

Classical Dynamics

Ground-state $n = 0$, the first excited state $n = 1$

Macroscopic occupation: use c-numbers $\beta_{0,1}$ for operators $b_{0,1}$

The occupation number has no definite value, its conjugate phase is well defined

These are coherent states defined by $b_{0,1} \left|\beta_{0,1}\right\rangle = \beta_{0,1} \left|\beta_{0,1}\right\rangle$

$\varepsilon_1 - \varepsilon_0 = \hbar\omega_0$, where $\omega_0 = ck_0$

Limit the wavevectors to the basic reciprocal vectors $\mathbf{k}_r$ of magnitude $k_r = k_0 = 2\pi/\lambda_0$

Use c-numbers α for the photon operators $a_{\alpha\mathbf{k}_r}$

$$L_{int} = \sqrt{\frac{2\pi\hbar}{V\omega_0}} J_{01} \left(\alpha + \alpha^*\right) \left(\beta_1^* \beta_0 + \beta_1 \beta_0^*\right)$$

$$L_f = \frac{\hbar}{4\omega_0} \left(\dot{\alpha}^2 + \dot{\alpha}^{*2} + 2\left|\dot{\alpha}\right|^2\right) - \frac{\hbar\omega_0}{4} \left(\alpha^2 + \alpha^{*2} + 2\left|\alpha\right|^2\right)$$

$$L_s = \frac{1}{2} i\hbar \left(\beta_0^* \dot{\beta}_0 - \dot{\beta}_0^* \beta_0 + \beta_1^* \dot{\beta}_1 - \dot{\beta}_1^* \beta_1\right) - \left(\varepsilon_0 \left|\beta_0\right|^2 + \varepsilon_1 \left|\beta_1\right|^2\right)$$

$$L_{int} = \frac{g}{\sqrt{N}} \left(\alpha + \alpha^*\right) \left(\beta_0 \beta_1^* + \beta_1 \beta_0^*\right)$$

$$g = \sqrt{\pi\hbar/6a^3\omega_0}J_{01} = \sqrt{\pi\hbar\omega_0(e^2/6a_0)}(a_0/a)^{3/2}$$

$$\varepsilon_1 - \varepsilon_0 = \hbar\omega_0 = 10eV,\ \lambda_0 = 10^3\text{Å},\ g \sim 0.8eV\ \ (a_0 = 0.53\text{Å})$$

Equations of Motion

$$\ddot{A} + \omega_0^2 A = \frac{2\omega_0 g}{\hbar\sqrt{N}}\left(\beta_0\beta_1^* + \beta_1\beta_0^*\right)$$

$$i\hbar\dot{\beta}_0 = \varepsilon_0\beta_0 - \frac{g}{\sqrt{N}}A\beta_1$$

$$i\hbar\dot{\beta}_1 = \varepsilon_1\beta_1 - \frac{g}{\sqrt{N}}A\beta_0$$

The Hamiltonian:

$$H_f = \frac{\hbar}{4\omega_0}\dot{A}^2 + \frac{\hbar\omega_0}{4}A^2$$

$$H_s = \varepsilon_0 \left|\beta_0\right|^2 + \varepsilon_1 \left|\beta_1\right|^2$$

$$H_{int} = -\frac{g}{\sqrt{N}}A\left(\beta_0\beta_1^* + \beta_1\beta_0^*\right)$$

Conservation laws:

$$H_f + H_s + H_{int} = E\ ,\ \left|\beta_0\right|^2 + \left|\beta_1\right|^2 = N$$

Solutions: Ground-State $\beta_{0,1} = B_{0,1} e^{i\Omega t}$

$$A = \tfrac{2g}{\hbar\omega_0}\sqrt{N}\left[1 - (\hbar\omega_0/2g)^4\right]^{1/2}$$

$$B_0^2 = \tfrac{1}{2}N\left[1 + (\hbar\omega_0/2g)^2\right]$$

$$B_1^2 = \tfrac{1}{2}N\left[1 - (\hbar\omega_0/2g)^2\right]$$

$$\Omega = \omega_0\left[-\frac{1}{2} + \frac{2g^2}{\hbar^2\omega_0^2}\right]$$

Critical coupling:

$$g > g_{cr} = \hbar\omega_0/2$$

Ground-state energy:

$$E = -\frac{g^2}{\hbar\omega_0} N \left[1 - (\hbar\omega_0/2g)^2\right]^2 = -\hbar\Omega B_1^2$$

Some consequences

Electric field vanishing

Magnetic field quite high $H \sim \sqrt{\hbar\omega_0/a^3} \sim 10^6 Gs$

Polarization $\mathbf{P} = \frac{1}{V}\sum_i \mathbf{p}(i)\cos\left(\theta_{1i} - \theta_{0i}\right)\left[1 - (\hbar\omega_0/2g)^4\right]^{1/2}$

Elementary excitations

$A \to A + \delta A$, $\beta_{0,1} \to \beta_{0,1} + \delta\beta_{0,1}$, $\delta\beta_{0,1} = \left(\delta B_{0,1} + iB_{0,1}\delta\theta_{0,1}\right) e^{i\Omega t}$

Solutions of the form $(\delta A, \delta B_1, \delta\varphi)e^{i\omega t}$

$$\omega_{1,2}^2 = \frac{1}{2}\omega_0^2 \left[\lambda^4 + 1 \pm \sqrt{\left(\lambda^4 - 1\right)^2 + 4}\right] \text{ , } \lambda = 2g/\hbar\omega_0$$

Elementary excitations $\Omega_{1,2} = \Omega \pm \omega_{1,2}$

Weak coupling limit these frequencies behave as $\omega_1 \simeq \sqrt{2}\omega_0$ and $\omega_2 \simeq \sqrt{\lambda^2 - 1}\omega_0$ $(\Omega_{1,2} \simeq \omega_{1,2})$.

Thermodynamics

No thermodynamics

$$Z \simeq tre^{\beta(\mu N - H)} = \int d\rho \cdot \frac{e^{\beta N \mu \rho}}{\sqrt{\hbar\omega_0 \left(\hbar\omega_0 - \mu\right) - 4g^2 \varrho}} \simeq e^{\beta N \mu \hbar\omega_0 (\hbar\omega_0 - \mu)/4g^2}$$

(Compute tr by $\int d\beta_{0x} d\beta_{0y} \ldots$)

Thermodynamic potential $\Omega = N\mu\hbar\omega_0 \left(\hbar\omega_0 - \mu\right)/4g^2$

Ordered phase, vanishing entropy

Super-Radiant Phase Transition

$$H_f = \hbar\omega_0 \sum_\mu \left(a^*_\mu a_\mu + 1/2\right) \ , \ H_s = \hbar\omega_0 b^*_1 b_1$$

$$H_{int} = -\frac{1}{\sqrt{N}} \left(G b^*_1 b_0 + G^* b^*_0 b_1\right)$$

μ stands for the pair $\alpha\mathbf{k}_r$, $G = \sum_\mu g_\mu a_\mu$ and $g_\mu = \sqrt{2\pi\hbar/V\omega_0} J_{01} N(\mu)/\sqrt{N}$

Compute the partition function by introducing spin variables

$$S_z = b^*_0 b_0 - b^*_1 b_1 = \sum_i \left(b^*_{0i} b_{0i} - b^*_{1i} b_{1i}\right) = \sum_i s_{zi}$$

$$S_+ = b^*_0 b_1 = \sum_i b^*_{0i} b_{1i} = \sum_i s_{+i}$$

$$S_- = b^*_1 b_0 = \sum_i b^*_{1i} b_{0i} = \sum_i s_{-i}$$

Free ensemble for $g < \hbar\omega_0$, at any temperature

For $g > \hbar\omega_0$ there exists a critical temperature T_c given by $\hbar^2\omega_0^2/g^2 = \tanh\beta_c\hbar\omega_0/2$ (or $\beta_c \simeq 2\hbar\omega_0/g^2$)

For $T > T_c$ free ensemble, for $T < T_c$ a non-trivial thermodynamics

In the former case the ensemble of particles is in the normal state, with a free energy per particle

$$f_0 = \hbar\omega_0/2 - \beta^{-1}\ln\left[2\cosh\beta\hbar\omega_0/2\right]$$

For T slightly below T_c the free energy per particle is

$$f \simeq f_0 - \frac{\hbar\omega_0}{4}(1 - T/T_c)^2$$

The entropy is continuous at the critical temperature

The specific heat has a discontinuity $C = C_0 + \hbar\omega_0/2T_c$

The transition is of the second kind, with the order parameter the photon occupation number

Conclusions

A new state of matter interacting with EM radiation

Macroscopic occupation of the atomic, molecular energy levels

Macroscopic occupation of the photon field, classical field

All due to a correlation between the internal phases and spatial positions

Pattern: coherence domains

Providing certain critical conditions on the coupling strength, temperature

New collective excitations, measurable