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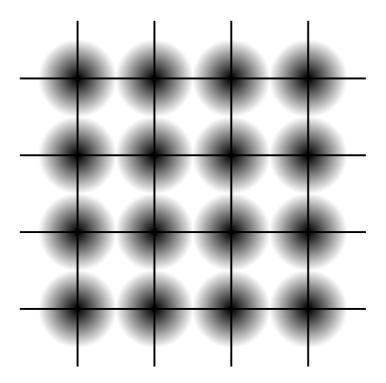
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COHERENCE DOMAINS in MATTER INTERACTING with RADIATION

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- 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!

Vector potential

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

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

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

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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:

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

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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:

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

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Matter Field (Substance)

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

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

Wavefunctions:

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

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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:

$$\Psi = \sum_{n} b_n \psi_n$$

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

$$N = \sum_{n} b_n^* b_n$$

The Lagrangian:

$$L_{s} = \frac{1}{2} \int d\mathbf{r} \left(\Psi^{*} \cdot i\hbar \partial \Psi / \partial t - i\hbar \partial \Psi^{*} / \partial t \cdot \Psi \right) - \int d\mathbf{r} \Psi^{*} H_{s} \Psi$$
$$L_{s} = \frac{1}{2} \sum_{n} i\hbar \left[b_{n}^{*} \dot{b}_{n} - \dot{b}_{n}^{*} b_{n} \right] - \sum_{n} \varepsilon_{n} b_{n}^{*} b_{n}$$

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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:

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

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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):

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

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

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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 $i\mathbf{k}\mathbf{r}_i - i\left(\theta_{ni} - \theta_{mi}\right)$! 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 13

Again

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

Coherence condition:

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

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

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

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

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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

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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 $b_{0,1} |\beta_{0,1}\rangle = \beta_{0,1} |\beta_{0,1}\rangle$

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

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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 $a_{\alpha \mathbf{k}_r}$

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

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

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

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

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

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

Equations of Motion

$$\ddot{A} + \omega_0^2 A = \frac{2\omega_0 g}{\hbar\sqrt{N}} \left(\beta_0 \beta_1^* + \beta_1 \beta_0^*\right)$$
$$i\hbar \dot{\beta}_0 = \varepsilon_0 \beta_0 - \frac{g}{\sqrt{N}} A \beta_1$$
$$i\hbar \dot{\beta}_1 = \varepsilon_1 \beta_1 - \frac{g}{\sqrt{N}} A \beta_0$$

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The Hamiltonian:

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

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

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

Conservation laws:

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

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

$$A = \frac{2g}{\hbar\omega_0} \sqrt{N} \left[1 - (\hbar\omega_0/2g)^4 \right]^{1/2}$$
$$B_0^2 = \frac{1}{2} N \left[1 + (\hbar\omega_0/2g)^2 \right]$$
$$B_1^2 = \frac{1}{2} N \left[1 - (\hbar\omega_0/2g)^2 \right]$$

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

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

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Elementary excitations

$$A \to A + \delta A$$
, $\beta_{0,1} \to \beta_{0,1} + \delta \beta_{0,1}$, $\delta \beta_{0,1} = (\delta B_{0,1} + i B_{0,1} \delta \theta_{0,1}) e^{i\Omega t}$
Solutions of the form $(\delta A, \delta B_1, \delta \varphi) e^{i\omega t}$

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

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

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

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

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

Ordered phase, vanishing entropy

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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

$$S_z = b_0^* b_0 - b_1^* b_1 = \sum_i (b_{0i}^* b_{0i} - b_{1i}^* b_{1i}) = \sum_i s_{zi}$$

$$S_+ = b_0^* b_1 = \sum_i b_{0i}^* b_{1i} = \sum_i s_{+i}$$

$$S_- = b_1^* b_0 = \sum_i b_{1i}^* b_{0i} = \sum_i s_{-i}$$

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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

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

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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

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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

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