# 221B Lecture Notes Quantum Field Theory III (Radiation Field)

# 1 Quantization of Radiation Field

Early development of quantum mechanics was led by the fact that electromagnetic radiation was quantized: photons. Now that we have gone through quantization of a classical field (Schrödinger field so far), we can proceed to quantize the Maxwell field. The basic idea is pretty much the same, except that there are subtletites associated with the gauge invariance of the vector potential.

#### 1.1 Classical Maxwell Field

The vector potential  $\vec{A}$  and the scalar potential  $\phi$  are combined in the four-vector potential

$$A^{\mu} = (\phi, \vec{A}). \tag{1}$$

Throughout the lecture notes, we use the convention that the metrix  $g_{\mu\nu} = \text{diag}(+1, -1, -1, -1)$  and hence  $A_{\mu} = g_{\mu\nu}A^{\nu} = (\phi, -\vec{A})$ . The four-vector coordinate is  $x^{\mu} = (ct, \vec{x})$ , and correspondingly the four-vector derivative is  $\partial_{\mu} = (\frac{1}{c}\frac{\partial}{\partial t}, \vec{\nabla})$ . The field strength is defined as  $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$ , and hence  $F_{0i} = \partial_{0}A_{i} - \partial_{i}A_{0} = -\vec{A}/c - \vec{\nabla}\phi = \vec{E}$ , while  $F_{ij} = \partial_{i}A_{j} - \partial_{j}A_{i} = -\vec{\nabla}_{i}A^{j} + \vec{\nabla}_{j}A^{i} = -\epsilon_{ijk}\vec{B}^{k}$ .

In the unit we have been using where the Coulomb potential is QQ'/r without a factor of  $1/4\pi\epsilon_0$ , the action for the Maxwell field is

$$S = \int dt d\vec{x} \left[ \frac{-1}{8\pi} F^{\mu\nu} F_{\mu\nu} - A_{\mu} j^{\mu} \right] = \int dt d\vec{x} \left[ \frac{1}{8\pi} \left( \vec{E}^2 - \vec{B}^2 \right) - A_{\mu} j^{\mu} \right].$$
(2)

I included a possible source term for the Maxwell field (electric current density)  $j^{\mu} = (\rho, \vec{j}/c)$ . For a point particle of charge e, the charge density is  $\rho = e\delta(\vec{x} - \vec{x}_0)$  while the current density is  $\vec{j} = e\vec{x}\delta(\vec{x} - \vec{x}_0)$ . They satisfy the current conversation law

$$\partial_{\mu}j^{\mu} = \frac{1}{c} \left( \frac{\partial}{\partial t} \rho + \vec{\nabla} \cdot \vec{j} \right) = 0.$$
(3)

The gauge invariance of the Maxwell field is that the vector potential  $A^{\mu}$  and  $A^{\mu} + \partial^{\mu}\omega$  (where  $\omega$  is an arbitrary function of spacetime) give the same field strength and hence the same action. Using this invariance, one can always choose a particular gauge. For most purposes of non-relativistic systems encountered in atomic, molecular, condensed matter, nuclear and astrophysics, Coulomb gauge is the convenient choice, while for highly relativistic systems such as in high-energy physics. We use Coulomb gauge in this lecture note:

$$\vec{\nabla} \cdot \vec{A} = 0. \tag{4}$$

A word of caution is that this gauge condition is not Lorentz-invariant, *i.e.*, the gauge condition is not frame independent. Therefore, when you go to a different frame of reference, you also need to perform a gauge transformation at the same time to preserve the Coulomb gauge condition. Another point is that, in the Coulomb gauge, the Gauss' law is

$$\vec{\nabla} \cdot \vec{E} = 4\pi j^0,\tag{5}$$

where  $j^0$  is the charge density. Because  $\vec{E} = -\vec{A} - \vec{\nabla}\phi$  and the Coulomb gauge condition, we find the Poisson equation

$$\Delta \phi = -4\pi\rho,\tag{6}$$

and hence

$$\phi(\vec{x},t) = \int d\vec{y} \frac{1}{|\vec{x} - \vec{y}|} \rho(\vec{y},t).$$
(7)

Note that the potential is not retarded, but instantaneous (*i.e.*, determined by the charge distribution at the same instance).

Hamiltonian for a particle of electric charge e in the presence of the Maxwell field is

$$H = \frac{(\vec{p} - \frac{e}{c}\vec{A})^2}{2m} + e\phi.$$
(8)

#### **1.2** Quantization

In order to quantize the Maxwell field, we first determine the "canonically conjugate momentum" for the vector potential  $\vec{A}$ . Following the definition  $p^i = \partial L/\partial \dot{q}^i$  in particle mechanics, we define the canonically conjugate momentum

$$\pi^{i} = \frac{\partial \mathcal{L}}{\partial \dot{A}^{i}} = -\frac{1}{4\pi c} E^{i} = \frac{1}{4\pi} \left( \frac{1}{c^{2}} \dot{A}^{i} + \frac{1}{c} \vec{\nabla}^{i} \phi \right).$$
(9)

In the absence of extremal sources, the scalar potential identically vanishes in Coulomb gauge (see Eq. (7)). We drop it entirely in this section.<sup>1</sup> Following the normal canonical commutation relation  $[q^i, p^j] = i\hbar\delta^{ij}$ , we set up the commutation relation

$$[A^{i}(\vec{x}), \pi^{j}(\vec{y})] = [A^{i}(\vec{x}), \frac{1}{4\pi c^{2}}\dot{A}^{j}(\vec{y})] = i\hbar\delta^{ij}\delta(\vec{x} - \vec{y}).$$
(10)

To satisfy this commutation relation, we introduce the photon creation and annihilation operators

$$[a^{i}(\vec{p}), a^{j\dagger}(\vec{q})] = \delta^{ij} \delta_{\vec{p}, \vec{q}}, \qquad (11)$$

and expand the vector potential and its time derivative as

$$A^{i}(\vec{x}) = \sqrt{\frac{2\pi\hbar c^{2}}{L^{3}}} \sum_{\vec{p}} \frac{1}{\sqrt{\omega_{p}}} (a^{i}(\vec{p})e^{i\vec{p}\cdot\vec{x}/\hbar} + a^{i\dagger}(\vec{p})e^{-i\vec{p}\cdot\vec{x}/\hbar})$$
(12)

$$\dot{A}^{i}(\vec{x}) = \sqrt{\frac{2\pi\hbar c^{2}}{L^{3}}} \sum_{\vec{p}} (-i\sqrt{\omega_{p}}) (a^{i}(\vec{p})e^{i\vec{p}\cdot\vec{x}/\hbar} - a^{i\dagger}(\vec{p})e^{-i\vec{p}\cdot\vec{x}/\hbar}).$$
(13)

Here,  $\omega_p = E_p/\hbar = c|\vec{p}|/\hbar$  is the angular frequency for the photon. You can check that this momentum-mode expansion together with the commutation relation Eq. (11) reproduces the canonical commutation relation Eq. (10) as follows.

$$\begin{split} &[A^{i}(\vec{x}), \dot{A}^{j}(\vec{y})] \\ &= \frac{2\pi\hbar c^{2}}{L^{3}} \sum_{\vec{p}, \vec{q}} (-i) [a^{i}(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar} + a^{i\dagger}(\vec{p}) e^{-i\vec{p}\cdot\vec{x}/\hbar}, a^{j}(\vec{p}) e^{i\vec{q}\cdot\vec{y}/\hbar} - a^{j\dagger}(\vec{q}) e^{-i\vec{q}\cdot\vec{y}/\hbar}] \\ &= \frac{2\pi\hbar c^{2}}{L^{3}} i \sum_{\vec{p}} \delta^{ij} (e^{i\vec{p}\cdot(\vec{x}-\vec{y})} + e^{-i\vec{p}\cdot(\vec{x}-\vec{y})}) \\ &= 4\pi\hbar c^{2} i \delta(\vec{x}-\vec{y}). \end{split}$$
(14)

At the last step, we used the correspondence in the large volume limit  $\sum_{\vec{p}} = L^3 \int d\vec{p}/(2\pi\hbar)^3$ .

The problem with what we have done so far is that we have not imposed the Coulomb gauge condition Eq. (4) on the vector potential yet. Acting the divergence on the momentum-mode expansion Eq. (12), we need

$$\vec{p} \cdot \vec{a}(\vec{p}) = 0. \tag{15}$$

<sup>&</sup>lt;sup>1</sup>Even when we have matter particles or fields, their charge density operator commutes with the vector potential, and hence the discussion here goes through unmodified.

The meaning of this equation is obvious: there is no longitudinal photon. There are only two transverse polarizations. To satisfy this constraint while retaining the simple commutation relations among creation and annihilation operators, we introduce the polarization vectors. When  $\vec{p} = (0, 0, p)$ , the positive helicity (right-handed) circular polarization has the polarization vector  $\vec{\epsilon}_+ = (1, i, 0)/\sqrt{2}$ , while the negative helicity (left-handed) circular polarization is represented by the polarization vector  $\vec{\epsilon}_- = (1, -i, 0)/\sqrt{2}$ . In general, for the momentum vector  $\vec{p} = p(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ , the circular polarization vectors are given by

$$\epsilon_{\pm}(\vec{p}) = \frac{1}{\sqrt{2}} \left( \pm \epsilon_1 + i\epsilon_2 \right), \tag{16}$$

where the linear polarization vectors are given by

$$\epsilon_1(\vec{p}) = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta), \tag{17}$$

$$\epsilon_2(\vec{p}) = (-\sin\phi, \cos\phi, 0). \tag{18}$$

Given the polarization vectors, we re-expand the vector potential in terms of the creation/annihilation operators

$$\begin{aligned}
A^{i}(\vec{x}) &= \sqrt{\frac{2\pi\hbar c^{2}}{L^{3}}} \sum_{\vec{p}} \frac{1}{\sqrt{\omega_{p}}} \sum_{\pm} (\epsilon^{i}_{\pm}(\vec{p})a_{\pm}(\vec{p})e^{i\vec{p}\cdot\vec{x}/\hbar} + \epsilon^{i}_{\pm}(\vec{p})^{*}a^{\dagger}_{\pm}(\vec{p})e^{-i\vec{p}\cdot\vec{x}/\hbar}) (19) \\
\dot{A}^{i}(\vec{x}) &= \sqrt{\frac{2\pi\hbar c^{2}}{L^{3}}} \sum_{\vec{p}} (-i\sqrt{\omega_{p}}) \sum_{\pm} (\epsilon^{i}_{\pm}(\vec{p})a_{\pm}(\vec{p})e^{i\vec{p}\cdot\vec{x}/\hbar} - \epsilon^{i}_{\pm}(\vec{p})^{*}a^{\dagger}_{\pm}(\vec{p})e^{-i\vec{p}\cdot\vec{x}/\hbar}).
\end{aligned}$$

(20)

With this expansion, the Coulomb gauge condition is automatically satisfied, while the creation/annihilation operators obey the commutation relations

$$[a_{\lambda}(\vec{p}), a^{\dagger}_{\lambda'}(\vec{q})] = \delta_{\lambda,\lambda'} \delta_{\vec{p},\vec{q}}$$
(21)

for  $\lambda, \lambda' = \pm$ . We could also have used the linearly polarized photons

$$\begin{aligned}
A^{i}(\vec{x}) &= \sqrt{\frac{2\pi\hbar c^{2}}{L^{3}}} \sum_{\vec{p}} \frac{1}{\sqrt{\omega_{p}}} \sum_{\lambda=1}^{2} \left(\epsilon_{\lambda}^{i}(\vec{p})a_{\lambda}(\vec{p})e^{i\vec{p}\cdot\vec{x}/\hbar} + \epsilon_{\lambda}^{i}(\vec{p})a_{\lambda}^{\dagger}(\vec{p})e^{-i\vec{p}\cdot\vec{x}/\hbar}\right) \quad (22)\\
\dot{A}^{i}(\vec{x}) &= \sqrt{\frac{2\pi\hbar c^{2}}{L^{3}}} \sum_{\vec{p}} \left(-i\sqrt{\omega_{p}}\right) \sum_{\lambda=1}^{2} \left(\epsilon_{\lambda}^{i}(\vec{p})a_{\lambda}(\vec{p})e^{i\vec{p}\cdot\vec{x}/\hbar} - \epsilon_{\lambda}^{i}(\vec{p})a_{\lambda}^{\dagger}(\vec{p})e^{-i\vec{p}\cdot\vec{x}/\hbar}\right).
\end{aligned}$$

$$(23)$$

with

$$[a_{\lambda}(\vec{p}), a^{\dagger}_{\lambda'}(\vec{q})] = \delta_{\lambda,\lambda'} \delta_{\vec{p},\vec{q}}$$
(24)

for  $\lambda, \lambda' = 1, 2$ . Clearly, two sets of operators are related by

$$a_1 = \frac{1}{\sqrt{2}}(a_+ + a_-), \qquad a_2 = \frac{i}{\sqrt{2}}(a_+ - a_-).$$
 (25)

Once we have the mode expansion for the vector potential, one can work out the Hamiltonian

$$H = \int d\vec{x} \frac{1}{8\pi} \left( \vec{E}^2 + \vec{B}^2 \right) = \sum_{\vec{p}} \sum_{\pm} \hbar \omega_p (a_{\pm}^{\dagger}(\vec{p}) a_{\pm}(\vec{p}) + \frac{1}{2}).$$
(26)

Because  $\hbar \omega_p = c |\vec{p}|$ , the dispersion relation for the photon is the familiar one  $E = c |\vec{p}|$  for a massless relativistic particle.

# 2 Classical Electromagnetic Field

Now that we found photons (particles) from the quantized radiation field, what is a classic electromagnetic field?

To answer this question, we study the quantum-mechanical Hamiltonian for the photons in the presence of a source. Starting from the action Eq. (2), we find the Hamiltonian

$$H = \int d\vec{x} \left[ \frac{1}{8\pi} \left( \vec{E}^2 + \vec{B}^2 \right) - \frac{1}{c} \vec{A} \cdot \vec{j} \right]$$
  
$$= \sum_{\vec{p},\lambda} \left( \hbar \omega_p a^{\dagger}_{\lambda}(\vec{p}) a_{\lambda}(\vec{p}) - \frac{1}{c} \sqrt{\frac{2\pi\hbar c^2}{L^3}} \frac{1}{\sqrt{\omega_p}} (\vec{\epsilon}_{\lambda}(\vec{p}) \cdot \vec{j}(\vec{p}) a_{\lambda}(\vec{p}) + \vec{\epsilon}^{*}_{\lambda}(\vec{p}) \cdot \vec{j}^{*}(\vec{p}) a^{\dagger}_{\lambda}(\vec{p})) \right). \quad (27)$$

Here, we omitted the zero-point energy because it is not relevant for the discussions below, and the Fourier modes of the source is defined by

$$\vec{j}(\vec{p}) \equiv \int d\vec{x} \vec{j}(\vec{x}) e^{i\vec{p}\cdot\vec{x}/\hbar},\tag{28}$$

and  $\vec{j}^*(\vec{p}) = \vec{j}(-\vec{p})$ . The interesting point is that for each momentum  $\vec{p}$  and polarization state  $\lambda$ , the Hamiltonian Eq. (27) is of the type

$$\hbar\omega(a^{\dagger}a - f^*a - a^{\dagger}f), \qquad (29)$$

whose ground state is

$$\hbar\omega(a^{\dagger}a - f^*a - a^{\dagger}f)|f\rangle = -\hbar\omega f^*f|f\rangle.$$
(30)

In other words, the ground state of the Hamiltonian for photons in the presence of a source term is a coherent state  $|f\rangle \equiv \prod_{\vec{p},\lambda} |f_{\lambda}(\vec{p})\rangle$ , with

$$f_{\lambda}(\vec{p}) = \sqrt{\frac{2\pi\hbar}{L^3}} \frac{1}{\hbar\omega_p^{3/2}} \vec{\epsilon}_{\lambda}^* \cdot \vec{j}^*(\vec{p}).$$
(31)

The vector potential has an expectation value in the coherent state, given by

$$\langle f | A^{i}(\vec{x}) | f \rangle$$

$$= \sum_{\vec{p},\lambda} \sqrt{\frac{2\pi\hbar c^{2}}{L^{3}}} \frac{1}{\hbar\omega_{p}^{2}} (\vec{\epsilon}_{\lambda}^{i}(\vec{p}) f_{\lambda}(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar} + \vec{\epsilon}_{\lambda}^{i*}(\vec{p}) f_{\lambda}^{*}(\vec{p}) e^{-i\vec{p}\cdot\vec{x}/\hbar})$$

$$= \frac{2\pi\hbar}{L^{3}} \sum_{\vec{p}} \frac{c}{\hbar\omega_{p}^{2}} \left( j^{k*}(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar} \sum_{\lambda} \epsilon_{\lambda}^{i}(\vec{p}) \epsilon_{\lambda}^{k*}(\vec{p}) + c.c. \right).$$

$$(32)$$

Even though the expression is somewhat complicated, one can check that this expectation value satisfies

$$\vec{\nabla} \times \langle f | \vec{B} | f \rangle = -\Delta \langle f | \vec{A} | f \rangle = \frac{4\pi}{c} \vec{j}, \qquad (33)$$

using the identity

$$\sum_{\lambda} \epsilon^{i}_{\lambda}(\vec{p}) \epsilon^{j*}_{\lambda}(\vec{p}) = \delta^{ij} - \frac{p^{i}p^{j}}{\vec{p}^{2}}$$
(34)

together with the Coulomb gauge condition  $\vec{\nabla} \cdot \vec{A} = 0$ . Actually, the term proportional to  $\vec{p}^i$  is a gradient  $-i\hbar\nabla^i$  and hence gauge-dependent. Ignoring the gauge-dependent term, we find a simpler expression

$$\langle f | A^{k}(\vec{x}) | f \rangle = \frac{2\pi}{L^{3}} \sum_{\vec{p}} \frac{c}{\hbar \omega_{p}^{2}} \left( j^{k*}(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar} + c.c. \right)$$

$$= \frac{4\pi}{c} \frac{1}{L^{3}} \sum_{\vec{p}} \left( \frac{1}{\vec{k}^{2}} j^{k*}(\vec{p}) e^{i\vec{k}\cdot\vec{x}} + c.c. \right),$$
(35)

which shows manifestly that it is a solution to the Poisson equation in the wave vector space  $\Delta = -\vec{k}^2$ .

What we have learnt here is that the ground state for the photon Hamiltonian in the presence of a source is given by a coherent state, which has an expectation value for the vector potential. This expectation value is nothing but what we normally obtain by solving Maxwell's equations for the classical Maxwell's field.

The solution we obtained, however, is not a "radiation" because it does not propagate. We can produce a radiation by turning off the current instantaneously at t = 0. Classically, it corresponds to a non-static source which can radiate electromagnetic wave. Quantum mechanically, we can use the "sudden" approximation that the same state given above now starts evolving according to the free photon Hamiltonian without the source term from t = 0and on.

The time evolution of a coherent state is very simple. For the free Hamiltonian  $H = \hbar \omega a^{\dagger} a$ , the time evolution is

$$|f,t\rangle = e^{-iHt}e^{-f^*f/2}e^{fa^{\dagger}}|0\rangle$$

$$= e^{-f^*f/2}e^{-i\omega a^{\dagger}at}\sum_{n=0}^{\infty}\frac{f^n}{n!}(a^{\dagger})^n e^{i\omega a^{\dagger}at}e^{-i\omega a^{\dagger}at}|0\rangle$$

$$= e^{-f^*f/2}\sum_{n=0}^{\infty}\frac{f^n}{n!}\left(e^{-i\omega a^{\dagger}at}a^{\dagger}e^{i\omega a^{\dagger}at}\right)^n|0\rangle$$

$$= e^{-f^*f/2}\sum_{n=0}^{\infty}\frac{f^n}{n!}(a^{\dagger}e^{-i\omega t})^n|0\rangle$$

$$= |fe^{-i\omega t}\rangle.$$
(36)

In other words, the time evolution keeps a coherent state still a coherent state, but with a different eigenvalue for the annihilation operator  $fe^{-i\omega t}$ . Then the expectation value for the vector potential can also be written down right away:

$$\langle f, t | A^k(\vec{x}) | f, t \rangle = \frac{4\pi}{c} \frac{1}{L^3} \sum_{\vec{p}} \left( \frac{1}{\vec{k}^2} j^{k*}(\vec{p}) e^{i\vec{k}\cdot\vec{x} - i\omega_p t} + c.c. \right).$$
(37)

One can see that this vector potential describes a propagating electromagnetic wave in the vacuum because of the factor  $e^{i\vec{p}\cdot\vec{x}/\hbar}e^{-i\omega_p t} = e^{i(\vec{k}\cdot\vec{x}-c|\vec{k}|t)}$  with  $\vec{k} = \vec{p}/\hbar$  and  $\omega_p = c|\vec{k}|$ . The quantum mechanical state is still a coherent state with time-dependent eigenvalues for the annihilation operators. The analogy to Bose–Einstein condensate is intriguing. In the case of Bose–Einstein condensate, we have a collection of particles which can be described either in terms of particle Hamiltonian or quantized Schrödinger field. After the condensate develops, it cannot be described by the particle Hamiltonian anymore, but rather by a "unquantized" version of Schrödinger field. The system exhibits macroscopic coherence. For the case of an electromagnetic wave, it is normally described by a classical Maxwell field. But one can talk about photons which appear in quantized radiation field. Then the "unquantized" version of the Maxwell field exhibits the macrosopic coherence.

Therefore, as long as the amplitude for the Maxwell field is "large," the number–phase uncertainty relation can easily be satisfied while manifesting coherence, and the quantum state is well described by a classical field, namely the Maxwell field.

# 3 Interaction With Matter

Now that we know how we get photons, we would like to discuss how photons are emitted or absorbed by matter.

When I was taking quantum mechanics courses myself, I was very frustrated. You hear about motivations why you need to study quantum mechanics, and most (if not all) of the examples involve photons: Planck's law, photoelectric effect, Compton scattering, emission spectrum from atoms, etc. But the standard quantum mechanics is incapable of dealing with creation and annihilation of particles, as we had discussed already. Now that we have creation and annihilation operators for photons, we are in the position to discuss emission and absorption of photons due to their interaction with matter.

#### 3.1 Hamiltonian

In this section, we deal with matter with conventional quantum mechanics, while with photons with quantized radiation field. This formulation is appropriate for decays of excited states of atoms, for instance. To be concrete, let us consider a hydrogen-like atom and its interaction with photons. We start with the Hamiltonian

$$H = \frac{\vec{p}^2}{2m} - \frac{Ze^2}{r}.$$
 (38)

Obviously, this Hamiltonian does not contain photons nor their interaction with the electron. The correct Hamiltonian for us is

$$H = \frac{(\vec{p} - \frac{e}{c}\vec{A})^2}{2m} - \frac{Ze^2}{r} + \sum_{\vec{p},\lambda} \hbar\omega_p a^{\dagger}_{\lambda}(\vec{p})a_{\lambda}(\vec{p}).$$
(39)

The first term describes the interaction of the electron with the vector potential  $\vec{A}(\vec{x})$ . For instance, the motion of electron in the constant magnetic field is described by this Hamiltonian with  $A_x = -By/2$ ,  $A_y = Bx/2$ . For our purpose, however, the vector potential is not a function of  $\vec{x}$  alone, which is an operator for the position of electron, but also contains creation and annihilation operators for photons. We rewrite the Hamiltonian Eq. (39 in two pieces

$$H = H_0 + V = H_e + H_{\gamma} + V, \tag{40}$$

$$H_e = \frac{\overline{p^2}}{2m} - \frac{Ze^2}{r}, \qquad (41)$$

$$H_{\gamma} = \sum_{\vec{p},\lambda} \hbar \omega_p a_{\lambda}^{\dagger}(\vec{p}) a_{\lambda}(\vec{p})$$
(42)

$$V = -\frac{e}{c} \frac{\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}}{2m} + \frac{e^2}{c^2} \frac{\vec{A} \cdot \vec{A}}{2m}.$$
 (43)

We regard  $H_0$  as the unperturbed Hamiltonian, and V as a perturbation. It is useful to know that  $\vec{p} \cdot \vec{A} = \vec{A} \cdot \vec{p}$  in the Coulomb gauge because the difference is  $\vec{p} \cdot \vec{A} - \vec{A} \cdot \vec{p} = -i\hbar \vec{\nabla} \cdot \vec{A} = 0$ .

#### 3.2 Free Hamiltonian

In perturbation theory, we have to solve the unperturbed system exactly so that we can perturb around it. What are the eigenstates and energy eigenvalues of the unperturbed Hamitonian  $H_0$  in our case? The point here is that there is no communication between the electron in  $H_e$  and photons in  $H_{\gamma}$ . Therefore, all we need to know is the eigenstates and eigenvalues of two separate Hamiltonians. The full eigenstates are product of two eigenstates, and the eigenvalues sum of two eigenvalues. For instance, we can consider states such as

$$\begin{aligned} &|1s\rangle|0\rangle,\\ |3d\rangle a^{\dagger}_{\lambda_1}(\vec{p_1})a^{\dagger}_{\lambda_2}(\vec{p_2})a^{\dagger}_{\lambda_3}(\vec{p_3})a^{\dagger}_{\lambda_4}(\vec{p_4})|0\rangle,\\ &|k,l,m\rangle a_{\lambda}(\vec{p})|0\rangle, \end{aligned}$$

and so on. The first state with the ground state of the system, with electron in the 1s state and no photons. The second state has the electron in an excited 3d state, with four photons. The last state has the electron in the continuum state with the momentum  $\hbar k$  and angular momentum l, m together with a photon. Their eigenvalues are simply the sum of the electron energy and photon energy (energies).

Therefore, we have solved the unperturbed Hamiltonian  $H_0$  exactly.

#### **3.3** Dipole Transition Rates

The next step is to deal with the interaction Hamiltonian V. What we use is the Fermi's golden rule for transition rates

$$W_{fi} = \frac{1}{\hbar} |\langle f|V|i\rangle|^2 2\pi \delta(E_f - E_i)$$
(44)

to the lowest order in perturbation theory.

To be specific, let us consider the decay of 2p state to 1s by emission of a photon. In other words,

$$|i\rangle = |2p\rangle|0\rangle \tag{45}$$

$$|f\rangle = |1s\rangle |\vec{q}, \lambda\rangle, \tag{46}$$

where the one-photon state is defined by

$$|\vec{q},\lambda\rangle = a^{\dagger}_{\lambda}(\vec{q})|0\rangle. \tag{47}$$

Because the initial and final states differ by one in the number of photons, and the vector potential  $\vec{A}$  changes the number of photons by one,  $\vec{A}^2$  term in V cannot contribute. Therefore,

$$\langle f|V|i\rangle = -\frac{e}{c}\frac{1}{m}\langle f|\vec{p}\cdot\vec{A}(\vec{x})|i\rangle, \qquad (48)$$

where we used the Coulomb gauge  $\vec{p} \cdot \vec{A} = \vec{A} \cdot \vec{p}$ . Now we can expand the vector potential in the momentum modes Eq. (19)

$$A^{i}(\vec{x}) = \sqrt{\frac{2\pi\hbar c^{2}}{L^{3}}} \sum_{\vec{q'},\lambda'} \frac{1}{\sqrt{\omega_{q'}}} (\epsilon^{i}_{\lambda'}(\vec{q'})a_{\lambda'}(\vec{q'})e^{i\vec{q'}\cdot\vec{x}/\hbar} + \epsilon^{i}_{\lambda'}(\vec{q'})^{*}a^{\dagger}_{\lambda'}(\vec{q'})e^{-i\vec{q'}\cdot\vec{x}/\hbar})$$
(49)

with a word of caution.  $\vec{x}$  is an operator describing the position of the electron, while  $\vec{q'}$  is a dummy *c*-number variable you sum over (so is the helicity  $\lambda'$ ).  $\vec{p}$  in Eq. (48), on the other hand, is also an operator describing the momentum of the electron. Because the final state has a photon while the initial state doesn't, only the piece with creation operator contributes to the amplitude Eq. (48). Therefore,

$$\langle f|V|i\rangle = -\frac{e}{c}\frac{1}{m}\langle \vec{q},\lambda|\sqrt{\frac{2\pi\hbar c^2}{L^3}}\sum_{\vec{q'},\lambda'}\frac{1}{\sqrt{\omega_{q'}}}\vec{\epsilon}^*_{\lambda'}(\vec{q'})a^{\dagger}_{\lambda'}(\vec{q'})|0\rangle \cdot \langle 1s|\vec{p}e^{-i\vec{q'}\cdot\vec{x}/\hbar}|2p\rangle.$$
(50)

The photon part of the matrix is element is easy:

$$\langle \vec{q}, \lambda | a^{\dagger}_{\lambda'}(\vec{q'}) | 0 \rangle = \delta_{\vec{q}, \vec{q'}} \delta_{\lambda, \lambda'} \tag{51}$$

and the summation over  $\vec{q'}$ ,  $\lambda'$  goes away. (Note that we can also easily deal with stimulated emission by having N photons in the initial state and N+1 photons in the final state, and the stimulated emission factor of  $\sqrt{N}$  in the amplitude comes out automatically.) Now the amplitude Eq. (50) reduces to

$$\langle f|V|i\rangle = -\frac{e}{c}\frac{1}{m}\sqrt{\frac{2\pi\hbar c^2}{L^3}}\frac{1}{\sqrt{\omega_q}}\vec{\epsilon}^*_{\lambda}(\vec{q})\cdot\langle 1s|\vec{p}e^{-i\vec{q}\cdot\vec{x}/\hbar}|2p\rangle.$$
(52)

Next, we point out that the exponential factor can be dropped as a good approximation. A higher order term in  $\vec{q} \cdot \vec{x}/\hbar$  is of order of magnitude of the size of the electron wave function  $a_0 = \hbar^2/Zme^2 = \hbar c/\alpha mc^2$  times the energy of the photon  $E_{\gamma} = E_{2p} - E_{1s} = \frac{1}{2}Z^2\alpha^2mc^2(1-\frac{1}{2^2})$  divided by c,  $|\vec{q}| = E_{\gamma}/c$ , and is hence suppressed by a factor of  $Z\alpha$ . This factor is small for a typical hydrogen-like atom. Finally, we use the identity

$$[H_e, \vec{x}] = -i\hbar \frac{\vec{p}}{m},\tag{53}$$

and hence

$$\langle 1s|\vec{p}|2p\rangle = i\frac{m}{\hbar}\langle 1s|[H_e,\vec{x}]|2p\rangle = i\frac{m}{\hbar}(E_{1s} - E_{2p})\langle 1s|\vec{x}|2p\rangle = -i\frac{m}{\hbar}E_\gamma\langle 1s|\vec{x}|2p\rangle.$$
(54)

It is customary to write the last factor in terms of the electric dipole operator

$$\vec{D} = e\vec{x},\tag{55}$$

and hence the transition amplitude Eq. (52) is

$$\langle f|V|i\rangle = \frac{i}{\hbar} |\vec{q}| \sqrt{\frac{2\pi\hbar c^2}{L^3}} \frac{1}{\sqrt{\omega_q}} \vec{\epsilon}^*_{\lambda}(\vec{q}) \cdot \langle 1s|\vec{D}|2p\rangle.$$
(56)

Because the transition amplitude is given in terms of the matrix element of the electric dipole operator, it is called the dipole transition.

Back to Fermi's golden rule Eq. (44), we now find

$$W_{fi} = \frac{1}{\hbar} \frac{1}{\hbar^2} \vec{q}^2 \frac{2\pi\hbar c^2}{L^3} \frac{1}{\omega_q} |\vec{\epsilon}^*_{\lambda}(\vec{q}) \cdot \langle 1s | \vec{D} | 2p \rangle|^2 2\pi \delta(E_f - E_i).$$
(57)

When one is interested in the total decay rate of the 2p state, we sum over all possible final states, namely the polarization and momentum of the photon. The decay rate of the 2p state is then

$$W_{i} = \sum_{\vec{q},\lambda} \frac{|\vec{q}|}{\hbar^{2}c} \frac{2\pi\hbar c^{2}}{L^{3}} |\vec{\epsilon}_{\lambda}^{*}(\vec{q}) \cdot \langle 1s|\vec{D}|2p\rangle|^{2} 2\pi\delta(E_{f} - E_{i})$$
  
$$= \int \frac{d\vec{q}}{(2\pi\hbar)^{3}} \frac{2\pi c|\vec{q}|}{\hbar} \sum_{\lambda} |\vec{\epsilon}_{\lambda}^{*}(\vec{q}) \cdot \langle 1s|\vec{D}|2p\rangle|^{2} 2\pi\delta(E_{f} - E_{i}).$$
(58)

Here we used the large volume limit  $\sum_{\vec{q}} = L^3 \int d\vec{q} / (2\pi\hbar)^3$ .

The transition matrix element of the electric dipole operator can be obtained easily. For example, for m = 0 state, only the z-component of the dipole operator is non-vanishing because of the axial symmetry around the z-axis, and

$$\langle 1s|\vec{D}|2p, m=0\rangle = e \int_0^\infty r^2 dr d\Omega \frac{1}{a^3} 2e^{-r/a} Y_0^0 \frac{\sqrt{16}}{12} \frac{r}{a} e^{-r/2a} Y_1^0 r \cos\theta = e \frac{1}{\sqrt{2}} \frac{256}{243} a_{23} \frac{1}{(59)} e^{-r/a} Y_1^0 r \cos\theta$$

with  $a = a_0/Z$ . By taking the sum over the polarization states using the two linear polarization states Eq. (17), only the first one contributes. Note also that  $2\pi\delta(E_f - E_i) = 2\pi\delta(|\vec{q}| - (E_{2p} - E_{1s})/c)/c$  and hence

$$W_{i} = \int \frac{d\Omega_{q}}{(2\pi\hbar)^{3}} |\vec{q}|^{2} \frac{(2\pi)^{2} |\vec{q}|}{\hbar} \left| \epsilon_{z,1}(\vec{q}) e \frac{1}{\sqrt{2}} \frac{256}{243} a \right|^{2}$$

$$= \int \frac{d\Omega_q}{2\pi\hbar^4} |\vec{q}|^3 \left( e \frac{1}{\sqrt{2}} \frac{256}{243} a \right)^2 \sin^2 \theta$$
  
$$= \frac{2}{3} \left( \frac{256}{243} \right)^2 e^2 \frac{q^3 a^2}{\hbar^4}$$
  
$$= \frac{256}{6561} Z^4 \alpha^5 \frac{mc^2}{\hbar}$$
  
$$= 6.27 \times 10^8 \text{sec}^{-1} Z^4. \tag{60}$$

In other words, the lifetime of the 2p state of hydrogen atom is  $W_i^{-1} = 1.60 \times 10^{-9}$  sec.

It is interesting to think about  $\sin \theta$  behavior of the amplitude. The reason behind it is fairly simple. Because we took m = 0 state as the initial state, there is no spin along the z-axis. On the other hand, in the final state, the atom does not carry spin (s-state) and the only carrier of spin is the photon. And the spin of the photon is always along the direction of its motion, either parallel (helicity +1) or anti-parallel (helicity -1). If the photon was emitted along the z-axis, there is net spin along the positive z-axis in the final state,  $\pm 1$  for the helicity  $\pm 1$  of the photon. To conserve angular momentum, such an amplitude should vanish identically, which is done precisely by  $\sin \theta = 0$  at  $\theta = 0$ . Photon emission along the negative z-axis must be likewise forbidden, by  $\sin \theta = 0$  at  $\theta = \pi$ . The m = 0 state has its angular momentum l = 1oriented in the x-y plane, which matches the helicity of the photon when emitted at  $\theta = \pi/2$ , causing the maximum amplitude in  $\sin \theta = 1$ . Because the algebra is somewhat lengthy, albeit straightforward, it always helps to have a simple understanding of the result based on intuitive arguments.

Now that we know the 2p state can decay into 1s state by emitting a photon (not that we didn't know it but now we can calculate it quantitatively), we can come back to the discussion we had with resonances in the scattering problem. When you consider the scattering of a photon with hydrogen atom in the 1s state, and when the photon energy is close to  $E_{2p} - E_{1s}$ , we can excite the atom to the 2p state, which decays later down to 1s state again. This causes a big enhancement in the photon-atom scattering crosss section. We had studied this phenomenon in the context of potential scattering before, and had identified such an enhancement as a consequence of a resonance. We had also learned back then that the energy of a resonance is slightly shifted downward on the complex plane, namely the energy has a negative imaginary part. How do we see that for the 2p state here?

The answer is quite simple. When you calculate a shift in the energy

eigenvalue at the second order in perturbation theory, the formula is

$$\Delta E = \sum_{f} \frac{\langle i|V|f\rangle\langle f|V|i\rangle}{E_i - E_f}.$$
(61)

Here, *i* is the state of your interest  $(|2p\rangle)$  in our case) and *f* runs over all possible intermediate states  $(|1s\rangle|\vec{q},\lambda\rangle)$  in our case). However, when the intermediate state is a continuum,  $E_i$  and  $E_f$  can in general be exactly the same. That would cause a singularity. To avoid it, we take the same prescription as we took in Lippmann–Schwinger equation to insert a factor of  $i\epsilon$ :

$$\Delta E = \sum_{f} \frac{\langle i|V|f\rangle\langle f|V|i\rangle}{E_i - E_f + i\epsilon}.$$
(62)

Having done that, we now write the denominator factor in the standard way as

$$\frac{1}{E_i - E_f + i\epsilon} = \mathcal{P}\frac{1}{E_i - E_f} - i\pi\delta(E_i - E_f).$$
(63)

Therefore the energy shift now has an imaginary part! We find

$$\Im \Delta E = -\pi \sum_{f} \langle i | V | f \rangle \langle f | V | i \rangle \delta(E_i - E_f).$$
(64)

You can see that it is related to Fermi's golden rule by

$$-\frac{\Gamma_i}{2} \equiv \Im \Delta E = -\frac{1}{2}\hbar \sum_f W_{fi} = -\frac{1}{2}\hbar W_i, \tag{65}$$

and hence the imaginary part of the energy is related to the decay rate of the unstable state (resonance) precisely in the way we discussed in the scattering theory.  $\Gamma$  is the HWFM of the Breit–Wigner resonance shape as a function of the energy, while  $\tau \equiv 1/W_i = \hbar/\Gamma_i$  is the lifetime of the resonance.

## 4 Multi-Pole Expansion

In many applications, it is useful to consider photons in angular-momentum eigenstates. This is equivalent to the multi-pole expansion of electromagnetic field.

#### 4.1 Spinless Schrödinger Field

First of all, the multi-pole expansion of the Schrödinger field  $\psi(\vec{x})$  without spin is given by the Laplace equation

$$(\Delta + k^2)\psi(\vec{x}) = \left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2\right)\psi(\vec{x}) = 0.$$
 (66)

The solutions regular at the origin are

$$u_{klm}(\vec{x}) = 2j_l(kr)Y_l^m(\theta,\phi).$$
(67)

It is normalized as

$$\int d\vec{x} u_{klm} u_{k'l'm'}^* = \delta_{ll'} \delta_{mm'} \frac{2\pi}{k^2} \delta(k - k').$$
(68)

Expanding a field in terms of angular momentum eigenmodes is the multipole expansion:

$$\psi(\vec{x}) = \sum_{lm} \int \frac{dk}{2\pi} k^2 a_{klm} u_{klm}(\vec{x}).$$
(69)

The canonical commutation relation  $[\psi(\vec{x}), \psi^{\dagger}(\vec{y})] = \delta(\vec{x} - \vec{y})$  implies the commutation relation

$$[a_{klm}, a^{\dagger}_{k'l'm'}] = \delta_{ll'} \delta_{mm'} \frac{2\pi}{k^2} \delta(k - k').$$
(70)

This set of creation and annihilation operators obey delta-function normalization because we have not put the system in a box. Correspondingly, a state created by the creation operator also satisfies the delta-function normalization

$$\langle k'l'm'|klm\rangle = \langle 0|a_{k'l'm'}a^{\dagger}_{klm}|0\rangle = \delta_{ll'}\delta_{mm'}\frac{2\pi}{k^2}\delta(k-k').$$
(71)

#### 4.2 Vector Potential

How do we expand a vector potential? We certainly need to find vectors out of  $u_{klm}$ . We do so by acting certain differential operators. Define<sup>2</sup>

$$\vec{u}_{kjm}^L = \frac{1}{k} \vec{\nabla} u_{kjm} \tag{72}$$

<sup>&</sup>lt;sup>2</sup>In 210B notation,  $X_{\ell m}^{(\ell)}$  corresponds to my  $\vec{u}_{klm}^M$  except that X does not seem to include the radial part.  $Z_{\ell m}$  corresponds to my  $\vec{u}_{klm}^E$  up to normalization factors. I could not rely on the notes, however, because he did not seem to have discussed the vector potential which we need for our purposes.

$$\vec{u}_{kjm}^M = \frac{1}{\sqrt{l(l+1)}} (\vec{x} \times \vec{\nabla}) u_{kjm}$$
(73)

$$\vec{u}_{kjm}^E = \frac{1}{k\sqrt{l(l+1)}} \vec{\nabla} \times (\vec{x} \times \vec{\nabla}) u_{kjm}.$$
(74)

Due to the reason we will see below, they are longitudinal, magnetic, and electric multipoles, respectively. They all satisfy the Laplace equation Eq. (66) because the differential operators acting on  $u_{kjm}$  all commute with the Laplacian. They also satisfy the normalization

$$\int d\vec{x} \vec{u}_{kjm}^A \cdot \vec{u}_{k'j'm'}^{B*} = \delta_{AB} \delta_{ll'} \delta_{mm'} \frac{2\pi}{k^2} 2\pi \delta(k - k'), \tag{75}$$

for A, B = L, E, M. Given this orthonormal set, we expand the vector potential as

$$\vec{A} = \sum_{lm} \sum_{A} \int \frac{dk}{2\pi} k^2 \sqrt{\frac{2\pi\hbar c^2}{\omega}} (a^A_{kjm} \vec{u}^A_{kjm} + a^{A\dagger}_{kjm} \vec{u}^{A*}_{kjm}),$$
(76)

and correspondingly,

$$\dot{\vec{A}} = \sum_{lm} \sum_{A} \int \frac{dk}{2\pi} k^2 (-i) \sqrt{2\pi\hbar c^2 \omega} (a^A_{kjm} \vec{u}^A_{kjm} - a^{A\dagger}_{kjm} \vec{u}^{A*}_{kjm}),$$
(77)

The creation and annihilation operators satisfy the commutation relation

$$[a_{kjm}^A, a_{kjm}^{A\dagger}] = \delta_{AB} \delta_{ll'} \delta_{mm'} \frac{2\pi}{k^2} \delta(k - k').$$
(78)

You can check the commutation relation Eq. (10) with this multipole expansion.

In the Coulomb gauge, we simply drop A = L from the summation because

$$\vec{\nabla} \cdot \vec{u}_{kjm}^L = \frac{1}{k} \Delta u_{kjm} = -k u_{kjm} \neq 0, \tag{79}$$

and hence does not satisfy the gauge condition. Electric and magnetic multipoles satisfy the Coulomb gauge condition.

The reason behind the names is very simple. Electric (magnetic) multipoles have non-vanishing radial component of electric (magnetic) field, while magnetic (electric) multipoles don't. Both  $u_{kjm}^{\vec{M},E}$  describes a mode with total

angular momentum j, with parity  $(-1)^{j+1}$  for magnetic and  $(-1)^j$  for electric multipoles (we will see this in the next section). An important point is that both multipoles vanish identically when j = 0, and hence a photon carries always angular momentum j = 1 or more. This is easy to see. The magnetic multipoles have basically the angular momentum operator acting on the spinless case  $u_{klm}^M = (\vec{x} \times \vec{\nabla})u_{klm} = \frac{i}{\hbar}\vec{L}u_{klm}$ . Therefore it is non-vanishing only when  $l \neq 0$ . The electric multipoles are curl of the magnetic ones, and again only non-vanishing ones are  $l \neq 0$ .

It may be confusing that I'm switching back and forth between j and l. Let us check what  $\vec{J} = \vec{L} + \vec{S}$  actually does on these modes.  $\vec{L} = -i\hbar(\vec{x} \times \vec{\nabla})$  is the usual one acting on the modes. (Note that we use  $\vec{L}$  or  $\vec{p}$  and their commutation relations in this discussion, but we only use them as short-hand notation for differential operators. They are not operators acting on the photon Fock space, but differential operators acting on the c-number mode functions  $\vec{u}_{klm}^A$  with which we are expanding the operator vector potential.) The spin matrices are obviously those for spin one case, and are given by

$$S_x = -i\hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad S_y = -i\hbar \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad S_z = -i\hbar \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
(80)

Note that  $\vec{u}_{kjm}^M = \frac{i}{\hbar} \vec{L} u_{klm}$ . Acting  $\vec{J}^2 = \vec{L}^2 + 2\vec{L} \cdot \vec{S} + \vec{S}^2$  on  $\vec{u}_{kjm}^M$ , we can see that  $\vec{L}^2 = l(l+1)\hbar^2$ , and  $\vec{S}^2 = 2\hbar^2$  because  $\vec{L}$  commutes with both of them. The action of  $\vec{L} \cdot \vec{S}$  needs to be worked out:

$$\vec{L} \cdot \vec{S} \vec{u}_{kjm}^{M} = -i\hbar \begin{pmatrix} 0 & L_z & -L_y \\ -L_z & 0 & L_x \\ L_y & -L_x & 0 \end{pmatrix} \frac{i}{\hbar} \begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} u_{klm}$$
$$= \begin{pmatrix} [L_z, L_y] \\ [L_x, L_z] \\ [L_y, L_x] \end{pmatrix} u_{klm}$$
$$= -\hbar^2 \vec{u}_{kjm}^{M}. \tag{81}$$

Therefore  $\vec{L} \cdot \vec{S} = -\hbar^2$ , and hence  $\vec{J}^2 = \vec{L}^2 + 2\vec{L} \cdot \vec{S} + \vec{S}^2 = l(l+1)\hbar^2 - 2\hbar^2 + 2\hbar^2 = l(l+1)\hbar^2$ . That is why  $u_{klm}$  gives the total angular momentum j = l, and we've used them interchangingly. It is also an eigenstate of the  $J_z = m\hbar$ ,

because

$$J_{z}\vec{u}_{kjm}^{M} = (L_{z} + S_{z})\frac{i}{\hbar} \begin{pmatrix} L_{x} \\ L_{y} \\ L_{z} \end{pmatrix} u_{klm}$$

$$= \frac{i}{\hbar} \begin{pmatrix} L_{z}L_{x} - i\hbar L_{y} \\ L_{z}L_{y} + i\hbar L_{x} \\ L_{z}L_{z} \end{pmatrix} u_{klm}$$

$$= \frac{i}{\hbar} \begin{pmatrix} L_{x}L_{z} \\ L_{y}L_{z} \\ L_{z}L_{z} \end{pmatrix} u_{klm}$$

$$= m\hbar \vec{u}_{kjm}^{M}.$$
(82)

It is not in a helicity eigenstate, however. The helicity is the spin along the direction of the momentum  $h = (\vec{S} \cdot \vec{p})/|\vec{p}|$ . If you act  $\vec{S} \cdot \vec{p}$  on  $\vec{u}_{klm}^M$ , you find

$$(\vec{S} \cdot \vec{p})\vec{u}_{kjm}^{M} = -i\hbar \begin{pmatrix} 0 & p_{z} & -p_{y} \\ -p_{z} & 0 & p_{x} \\ p_{y} & -p_{x} & 0 \end{pmatrix} \begin{pmatrix} L_{x} \\ L_{y} \\ L_{z} \end{pmatrix} u_{klm}$$
$$= \hbar^{2}\vec{\nabla} \times \vec{u}_{klm}^{M}$$
$$= \hbar^{2}k\vec{u}_{klm}^{E}.$$
(83)

The electric multipoles  $\vec{u}_{kjm}^E$  also have the eigenvalues  $\vec{J}^2 = l(l+1)\hbar^2$ ,  $J_z = m\hbar$ . That can be shown by the fact that  $\vec{u}_{klm}^E = (\vec{S} \cdot \vec{p})\vec{u}_{kjm}^M/\hbar^2 k$ , and that  $(\vec{S} \cdot \vec{p})$  commutes with  $\vec{J}$ . Acting  $(\vec{S} \cdot \vec{p})$  on  $\vec{u}_{kjm}^E$  brings back  $\vec{u}_{kjm}^M$ .

#### 4.3 Parity

Parity is the reflection of space:  $\vec{x} \to -\vec{x}$ . Another advantage of the multipole expansion is that the photon is not only in the angular momentum eigenstate but also in the parity eigenstate. The combination of them leads to useful selection rules in the transition amplitudes.

In quantum mechanics, parity P is a unitary and hermitean operator. Like any other symmetry operators such as translation, rotation, time evolution, etc, it has to be unitary  $PP^{\dagger} = 1$  to preserve the probabilities. But doing parity twice is the same as doing nothing, PP = 1. Then we find  $P = P^{\dagger}$ and hence it is hermitean. Therefore, states can be classified according to the eigenvalues of the parity operator. If the Hamiltonian is parity-invariant, PHP = H, it also means [P, H] = 0 (use  $P^2 = 1$ ) and hence the parity is conserved. In other words, if the initial state is an eigenstate of the parity, and final state also should have the same parity eigenvalue. For instance, a particle in a central potential is described by the Hamiltonian

$$H = \frac{\vec{p}^2}{2m} + V(r),$$
 (84)

which is parity invariant. To see this, we use the definition  $P\vec{x}P = -\vec{x}$ , and note that the canonical commutation relation  $[x^i, p^j] = i\hbar\delta^{ij}$  requires the momentum to also flip its sign  $P\vec{p}P = -\vec{p}$ . The radius  $r = |\vec{x}|$  of course doesn't change under parity. For convenience, I call the parity on the charged particle (say, electron)  $P_e$  instead of just P. This is because I need a separate parity acting on the vector potential below.

The parity on the vector potential is

$$P_{\gamma}\vec{A}(\vec{x})P_{\gamma} = -\vec{A}(-\vec{x}). \tag{85}$$

Under this transformation, the electric and magnetic fields transform as

$$P_{\gamma}\vec{E}(\vec{x})P_{\gamma} = -\vec{E}(-\vec{x}), \qquad P_{\gamma}\vec{B}(\vec{x})P_{\gamma} = \vec{B}(-\vec{x}). \tag{86}$$

It is easy to check that the Hamitonian of the radiation field is invariant under parity.

Finally, we look at the interaction Hamiltonian

$$\frac{(\vec{p} - \frac{e}{c}\vec{A}(\vec{x}))^2}{2m}.$$
(87)

Acting  $P_e$  makes it to

$$P_e \frac{(\vec{p} - \frac{e}{c}\vec{A}(\vec{x}))^2}{2m} P_e = \frac{(-\vec{p} - \frac{e}{c}\vec{A}(-\vec{x}))^2}{2m},$$
(88)

which is not the same. But further acting  $P_{\gamma}$  makes it to

$$P_{\gamma}P_{e}\frac{(\vec{p}-\frac{e}{c}\vec{A}(\vec{x}))^{2}}{2m}P_{e}P_{\gamma} = P_{\gamma}\frac{(-\vec{p}-\frac{e}{c}\vec{A}(\vec{-x}))^{2}}{2m}P_{\gamma} = \frac{(-\vec{p}+\frac{e}{c}\vec{A}(\vec{x}))^{2}}{2m} = \frac{(\vec{p}-\frac{e}{c}\vec{A}(\vec{x}))^{2}}{(89)}$$

and hence the Hamiltonian is invariant under the product  $P \equiv P_{\gamma}P_e$ . Therefore the parity eigenvalue that is conserved is the *product* of parity eigenvalues of electrons and photons.

Now we try to identify the parity of a photon in a multipole. The starting point is the property of the spherical harmonics

$$Y_{l}^{m}(\pi - \theta, \phi + \pi) = (-1)^{l} Y_{l}^{m}(\theta, \phi).$$
(90)

The argument  $(\pi - \theta, \phi + \pi)$  corresponds to the reflected position vector  $-\vec{x}$ . Based on this property, it is usually said that the state with orbital angular momentum l is an eigenstate of parity with the eigenvalue  $(-1)^l$ . The magnetic multipole mode function is defined by acting  $\vec{x} \times \vec{\nabla}$ , which is even under parity. Therefore,

$$\vec{u}_{kjm}^M(-\vec{x}) = (-1)^j \vec{u}_{kjm}^M(\vec{x}).$$
(91)

The electric multiple mode functions are obtained by taking curl of the magnetic ones, and therefore there is an additional sign under parity, and hence

$$\vec{u}_{kjm}^E(-\vec{x}) = (-1)^{j+1} \vec{u}_{kjm}^E(\vec{x}).$$
(92)

Now the right-hand side of Eq. (85) is

$$-\vec{A}(-\vec{x}) = -\sum_{jm} \int \frac{dk}{2\pi} k^2 (a^E_{jkm} \vec{u}^E_{jkm} (-\vec{x}) + a^M_{jkm} \vec{u}^M_{jkm} (-\vec{x}) + \text{h.c.})$$
  
$$= \sum_{jm} \int \frac{dk}{2\pi} k^2 ((-1)^j a^E_{jkm} \vec{u}^E_{jkm} (\vec{x}) + (-1)^{j+1} a^M_{jkm} \vec{u}^M_{jkm} (\vec{x}) + \text{h.c.}), \quad (93)$$

where h.c. stands for hermitean conjugate. On the other hand, the only operator in the multipole expansion of the vector potential is the creation and annihilation operators, and only they are affected by  $P_{\gamma}$ . The l.h.s of eq. (85) is then

$$P_{\gamma}\vec{A}(\vec{x})P_{\gamma} = \sum_{jm} \int \frac{dk}{2\pi} k^2 (P_{\gamma}a^E_{jkm}P_{\gamma}\vec{u}^E_{jkm}(\vec{x}) + P_{\gamma}a^M_{jkm}P_{\gamma}\vec{u}^M_{jkm}(\vec{x}) + \text{h.c.}).$$
(94)

Comparing Eqs. (94,93), we find

$$P_{\gamma}a_{jkm}^{E}P_{\gamma} = (-1)^{j}a_{jkm}^{E}, \qquad P_{\gamma}a_{jkm}^{M}P_{\gamma} = (-1)^{j+1}a_{jkm}^{M}.$$
(95)

The parity eigenvalues of photon states in a given multipole are

$$P_{\gamma}|jkm,E\rangle = P_{\gamma}a_{jkm}^{E\dagger}|0\rangle = (-1)^{j}a_{jkm}^{E\dagger}|0\rangle = (-1)^{j}|jkm,E\rangle, \qquad (96)$$

where I used  $P_{\gamma}|0\rangle = |0\rangle$ . Therefore the parity eigenvalue of a photon in electric multipoles is given by  $P_{\gamma} = (-1)^{j}$ . Similarly, they are  $P_{\gamma} = (-1)^{j+1}$  for photons in magnetic multipoles.

Conservation of parity provides powerful selection rules in many systems, especially atomic, molecular and nuclear transitions by emission or absorption of photons. This is because electromagnetism conserves parity. Until 1957, all forces in Nature were believed to conserve parity. The space looks symmetric between right and left, right? Of course! But in 1957, T.D. Lee and C.N. Yang pointed out that parity may be violated in weak interactions. Their study started with what was called  $\tau$ - $\theta$  puzzle. These particles were discovered in cosmic rays, later produced artificially in accelerators, and studied (mostly) in bubble chambers.  $\tau^+$  particle was identified by its decay into  $\pi^+$  and  $\pi^0$  (remember Yukawa's pions responsible for binding protons and neutrons in nuclei), while  $\theta^+$  into  $\pi^+\pi^+\pi^-$ . Because pions have odd intrinsic parity, and the decay is dominated by S-wave,  $\tau^+$  has even parity and  $\theta^+$  odd. The puzzle was that they appeared to have exactly the same mass and lifetime. It was too much of a coincidence that Nature provides two particles with identical mass and lifetime. Given this puzzle, Lee and Yang pointed out that maybe  $\tau^+$  and  $\theta^+$  are not separate particles which happen to have the same masses and lifetimes, but are a single particle with different decay modes. For this to be true, a particle must be decaying into final states with opposite parities, and hence the parity must be broken (i.e., not conserved). Then they asked the question how well parity conservation has been tested experimentally, and to surprise of many people, found that the parity conservation has been tested only in electromagetic and strong interactions, to some extent in gravity, but never in weak interactions which are responsible for nuclear  $\beta$ -decay and decay of  $\tau$  and  $\theta$  particles. They proposed various ways to test (or see violation of) parity in weak interactions. One of them was to study a possible correction between the spin of nucleus and the momentum of the  $\beta$ -electron. Under parity, spin remains the same while the momentum flips. Therefore, if there is any correlation between the spin and the momentum, it means parity is broken. This experiment was done soon after Lee–Yang's paper by C.S. Wu. She studied the  $\beta$  decay of <sup>60</sup>Co. She was clever to use the then-novel discovery that one can polarize nuclei in a magnetic field even when the temperature is not so low. Recall

that the nuclear magneton is 2000 times smaller than the Bohr magneton, and it appears it would require an extremely large magnetic field and low temperature to polarize nuclei. However, a magnetic field polarizes unpaired electrons in the atom, which in turn polarizes nuclei due to hyperfine interactions. This turned out to be a much more effective way to polarize nuclei. She still needed a cryostat of course. (I didn't look up the parameters.) She could demonstrate that the  $\beta$ -electrons are emitted preferentially parallel to the spin of the nucleus, while the preference slowly disappeared once she turned off the cryostat. Since then, we know that there is a fundamental distinction between left and right. The division in Congress has a deep root, indeed!

#### 4.4 Multipole Transitions

Emission of photons in  $\vec{u}_{kjm}^{E,M}$  is called Ej or Mj transitions. For instance, the electric dipole transition produces a photon in the state  $\vec{u}_{k1m}^E$ , and is called E1 transition. The coupling of a magnetic moment to magnetic field in the Hamiltonian can cause the emission of a photon by a M1 transition. Because  $j_l(kr) = (kr)^l/(2l+1)!!$  at small r, higher multipole transitions are suppressed by powers of kr, similarly to the reason why we could omit higher powers in  $\vec{q} \cdot \vec{x}/\hbar$  in the  $2p \to 1s$  E1 transition discussed above.

As an example, we recalculate the 2p to 1s transition using the multipole expansion. In this case, the angular momentum of the atom changes by one unit, which needs to be carried away by the photon. Therefore, only possibilities are E1 and M1 transitions. This way, you can see that the dipole transitions are the only possibilities even before doing any calculations; this is a big advantage in the multipole expansion. To proceed, we need the mode functions  $u^{M,E}$  for j = 1. We take  $|2p, m = 0\rangle$  again as the initial state, and hence the only mode functions we need are  $\vec{u}_{k10}^{M,E}$ . First,

$$\vec{u}_{k10}^{M} = \frac{i}{\hbar} \begin{pmatrix} L_x \\ L_y \\ L_z \end{pmatrix} 2j_1(kr)Y_1^0 \frac{1}{\sqrt{1(1+1)}} \\ = \frac{i}{\hbar} \begin{pmatrix} (L_+ + L_-)/2 \\ (L_+ - L_-)/2i \\ L_z \end{pmatrix} 2j_1(kr)Y_1^0 \frac{1}{\sqrt{2}}$$

$$= i \begin{pmatrix} (Y_1^1 + Y_1^{-1})/2 \\ (Y_1^1 - Y_1^{-1})/2i \\ 0 \end{pmatrix} 2j_1(kr) \frac{1}{\sqrt{2}} \\ = \sqrt{\frac{3}{2\pi}} \begin{pmatrix} \sin\theta\sin\phi \\ -\sin\theta\cos\phi \\ 0 \end{pmatrix} j_1(kr).$$
(97)

Using the behavior for small kr,  $j_1(kr) \simeq kr/3$ , we find

$$\vec{u}_{k10}^M \simeq \frac{k}{\sqrt{6\pi}} \begin{pmatrix} y \\ -x \\ 0 \end{pmatrix}.$$
(98)

On the other hand, the electric dipole mode is

$$\vec{u}_{k10}^E = \frac{1}{k} \vec{\nabla} \times \vec{u}_{k10}^M \simeq -\sqrt{\frac{2}{3\pi}} \begin{pmatrix} 0\\0\\1 \end{pmatrix}.$$
(99)

Note that there is no suppression due to kr in the electric dipole mode and hence is dominant over the magnetic dipole transition. (Another reason why the magnetic dipole transition is not important is because it is forbidden for  $2p \rightarrow 1s$  transition due to parity conservation. We actually know that before working out the mode function.) In general, magnetic multipole transitions are suppressed relative to the electric ones for the same multipole in nonrelativistic systems.

The only important piece in the multipole expansion of the vector potential is then

$$\vec{A}(\vec{x}) \ni \int_0^\infty \frac{dk}{2\pi} k^2 \sqrt{\frac{2\pi\hbar c^2}{\omega_k}} a_{k10}^\dagger \left(-\sqrt{\frac{2}{3\pi}}\right) \begin{pmatrix} 0\\0\\1 \end{pmatrix}.$$
 (100)

(I'm using a sloppy notation that  $\ni$  means the r.h.s. is only the important part of the l.h.s.) Then the interaction Hamiltonian is

$$V = -\frac{e}{c}\frac{1}{m}p_z A_z \ni \frac{e}{mc}\sqrt{\frac{2}{3\pi}}p_z \int_0^\infty \frac{dk}{2\pi}k^2 \sqrt{\frac{2\pi\hbar c^2}{\omega_k}}a_{k10}^{\dagger}.$$
 (101)

The matrix element is (see Eq. (59))

$$\langle 1s|\langle k10|V|0\rangle|2p, m = 0\rangle$$

$$= \frac{e}{mc}\sqrt{\frac{2}{3\pi}} \int_0^\infty \frac{dk'}{2\pi} k'^2 \sqrt{\frac{2\pi\hbar c^2}{\omega_{k'}}} \langle k10|a^{\dagger}_{k'10}|0\rangle \langle 1s|p_z|2p, m = 0\rangle$$

$$= \frac{e}{mc}\sqrt{\frac{2}{3\pi}} \sqrt{\frac{2\pi\hbar c^2}{\omega_k}} \frac{1}{\sqrt{2}} \frac{256}{243} a\frac{m}{\hbar} E_{\gamma}.$$
(102)

(Recall  $q = \hbar k = E_{\gamma}/c = \hbar \omega_k/c$ .)

The decay rate is again given by the Fermi's golden rule Eq. (44). The only non-trivial difference is that the summation over the final state is given by

$$\sum_{f} = \sum_{jm} \int \frac{dk}{2\pi} k^2, \qquad (103)$$

while only j = 1, m = 0 contributes in our case. Therefore,

$$W_{i} = \frac{1}{\hbar} \int \frac{dk}{2\pi} k^{2} \frac{e^{2}}{m^{2}c^{2}} \frac{2}{3\pi} \frac{2\pi\hbar^{2}c}{q} \left(\frac{1}{\sqrt{2}} \frac{256}{243}a\right)^{2} \frac{m^{2}}{\hbar^{2}} (cq)^{2} 2\pi\delta(E_{f} - E_{i})$$
  
$$= \frac{e^{2}}{\hbar^{4}} q^{3} a^{2} \frac{2}{3} \left(\frac{256}{243}\right)^{2}, \qquad (104)$$

which precisely agrees with Eq. (60).

As we have seen in this example, the advantage of the multipole expansion is that the selection rule is manifest. For a given initial and final state with fixed angular momenta and parities, one can immediately tell that multipole would dominate in the transition.

Bob Cahn mentioned an example in nuclear  $\gamma$  decay from a 2<sup>+</sup> state to a 5<sup>+</sup> state. From the angular momentum consideration, the photon must be in the multipoles of j = 3, 4, 5, 6, or 7. From the parity consideration, it has to have even parity. Therefore, allowed multipole transitions are M3, E4, M5, E6, M7. Higher multipoles have higher powers in kr and hence are suppressed. However, as we saw above, the electric multipoles have one less power in kr compared to the corresponding magnetic ones. Therefore, M3 and E4 transitions appear with the same power in kr (third power) and they both contribute in this transition and they interfere.

### 5 Casimir Effect

So far, we had not cared much about the zero-point energy of the photons in Eq. (26). It is often said that the zero-point energy just amounts to the baseline energy and all other energies are measured relative to it. In other words, pretending it doesn't exist is enough. But the zero-point energy plays a role if a change in the system affects the zero-point energy itself. (See Milonni, P. W., and Shih, M. L., 1992, *Contemp. Phys.* **33**, 313. for a review.)

To be concrete, put two conducting plates parallel to each other. The distance between the plates is d (at z = 0 and z = d), and the plates are very large of area  $L^2$  where we take  $L \to \infty$ . To simplify the discussions, we also place thin plates at x = 0, x = L and y = 0, y = L to form a box. A conducting plate imposes boundary conditions on the radiation field  $E_{\parallel} = 0$  and  $B_{\perp} = 0$ . Given these boundary conditions, the vector potential is expanded in modes as

$$\vec{A}(\vec{x}) \sim \vec{\epsilon} \sin(n_x, n_y, n_z) \left(\frac{\pi n_x}{L} x + \frac{\pi n_y}{L} y + \frac{\pi n_z}{d} z\right), \tag{105}$$

for  $n_x$ ,  $n_y$ , and  $n_z$  non-negative integers. For each wave vector  $\vec{k} = (\pi n_x/L, \pi n_y/L, \pi n_z/d)$ , the polarization vector is transverse:  $\vec{k} \cdot \vec{\epsilon} = 0$ . If one of the *n*'s vanishes, however, say  $\vec{k} = (0, \pi n_y/L, \pi n_z/d)$ , the polarization vector  $\vec{\epsilon} = (1, 0, 0)$  is not allowed because that would give  $A_x \neq 0$  for any *x* (and generic *y*, *z*) and violates the boundary condition  $E_{\parallel} = 0$ . Therefore, we have only one polarization whenever one of *n*'s vanishes.

The sum of zero point energies in this set up is therefore given by

$$U(d) = \sum' \frac{1}{2} \hbar \omega \times 2 = \sum_{n_x, n_y, n_z} \hbar c \left[ \left( \frac{\pi n_x}{L} \right)^2 + \left( \frac{\pi n_y}{L} \right)^2 + \left( \frac{\pi n_z}{d} \right)^2 \right]^{1/2}.$$
 (106)

The summation  $\Sigma'$  means that whenever one of *n*'s vanishes, we drop the multiplicity 2 for possible transverse polarizations. Because we regard the size of the plate to be large  $L \to \infty$ , we can replace the sum over  $n_x$ ,  $n_y$  in terms of integrals over  $k_{x,y} = \pi n_{x,y}/L$ ,

$$U(d) = \left(\frac{L}{\pi}\right)^2 \sum_{n_z} \int_0^\infty dk_x \int_0^\infty dk_y \hbar c \left[k_x^2 + k_y^2 + \left(\frac{\pi n_z}{d}\right)^2\right]^{1/2}.$$
 (107)

Recall that we are interested in the *difference* in the zero-point energy when d is varied. Therefore, it is useful to compare it to the case when the plates don't exist. We can compute the zero-point energy density in the infinite volume as usual, and then calcualte the energy  $U_0(d)$  multiplied by the volume  $L^2d$ :

$$U_{0}(d) = Ld^{2} \int \frac{d\vec{k}}{(2\pi)^{3}} \hbar c \left[k_{x}^{2} + k_{y}^{2} + k_{z}^{2}\right]^{1/2}$$
  
$$= Ld^{2} \int_{0}^{\infty} \frac{dk_{x}}{\pi} \int_{0}^{\infty} \frac{dk_{y}}{\pi} \int_{0}^{\infty} \frac{dk_{z}}{\pi} \hbar c \left[k_{x}^{2} + k_{y}^{2} + k_{z}^{2}\right]^{1/2}.$$
 (108)

What is observable is the difference

$$U(d) - U_{0}(d) = \frac{L^{2}}{\pi^{2}} \hbar c \int_{0}^{\infty} dk_{x} dk_{y} \left\{ \sum_{n_{z}} \left[ k_{x}^{2} + k_{y}^{2} + \left(\frac{\pi n_{z}}{d}\right)^{2} \right]^{1/2} - \frac{d}{\pi} \int_{0}^{\infty} dk_{z} \left[ k_{x}^{2} + k_{y}^{2} + k_{z}^{2} \right]^{1/2} \right\}.$$
(109)

Switching to the circular coordinates,

$$\int_0^\infty dk_x dk_y = \int_0^\infty k_\perp dk_\perp \int_0^{\pi/2} d\phi = \frac{\pi}{4} \int_0^\infty dk_\perp^2,$$

we find

$$U(d) - U_0(d) = \frac{L^2}{\pi^2} \hbar c \frac{\pi}{4} \int_0^\infty dk_\perp^2 \left\{ \sum_{n_z} \left[ k_\perp^2 + \left( \frac{\pi n_z}{d} \right)^2 \right]^{1/2} - \frac{d}{\pi} \int_0^\infty dk_z \left[ k_\perp^2 + k_z^2 \right]^{1/2} \right\}.$$
(110)

This expression appears problematic because it looks badly divergent. The divergence appears when the wave vector is large, which corresponds to high frequency photons. The point is that the conducting plates are transparent to, say, gamma rays, or in general for photons whose wavelengths are shorter than interatomic separation a. Therefore, there is naturally a damping factor  $f(\omega) = f(c(k_{\perp}^2 + k_z^2)^{1/2})$  with f(0) = 1 which smoothly cuts off the integral for  $\omega \gtrsim c/a$ . In particular,  $f(\infty) = 0$ . Then the expression is safe and allows

us to use standard mathematical tricks. Changing to dimensionless variables  $u = (k_{\perp}d/\pi)^2$  and  $n_z = k_z d/\pi$ ,

$$U(d) - U_0(d) = \frac{\pi^2 L^2 \hbar c}{4d^3} \int_0^\infty du \left\{ \sum_{n_z} \sqrt{u + n_z^2} - \int_0^\infty dn_z \sqrt{u + n_z^2} \right\} f(\omega).$$
(111)

Interchanging the sum and integral, we define the integral

$$F(n) = \int_0^\infty du\sqrt{u+n^2}f(\omega) = \int_{n^2}^\infty du\sqrt{u}f(\omega)$$
(112)

with  $\omega = \pi c \sqrt{u}/d$  in the last expression. Using this definition, we can write

$$U(d) - U_0(d) = \frac{\pi^2 L^2 \hbar c}{4d^3} \left\{ \frac{1}{2} F(0) + \sum_{n=1}^{\infty} F(n) - \int_0^{\infty} dn F(n) \right\}.$$
 (113)

Here we can use the Euler–McLaurin formula

$$\frac{1}{2}F(0) + \sum_{n=1}^{\infty} F(n) - \int_0^{\infty} F(n) = -\frac{1}{2!} B_2 F'(0) - \frac{1}{4!} B_4 F'''(0) - \cdots$$
(114)

The coefficientss  $B_k$  are Bernouilli numbers defined by the Taylor expansion

$$\frac{x}{e^x - 1} = \sum_{k=0}^{\infty} B_k \frac{x^k}{k!},$$
(115)

and  $B_0 = 1$ ,  $B_1 = -1/2$ ,  $B_2 = 1/6$ ,  $B_4 = -1/30$ , and all odd ones  $B_{2n-1}$  vanish except  $B_1$ .

Here is a physicist's proof of the Euler–McLaurin formula. Using the Taylor expansion that defines the Bernouilli numbers, we replace x to a derivative operator  $\partial_x$ 

$$\frac{\partial_x}{e^{\partial_x} - 1} = \sum_{k=0}^{\infty} B_k \frac{\partial_x^k}{k!}.$$
(116)

We act this operator on a function F(x) and integrate it over x from 0 to  $\infty$ ,

$$\int_0^\infty dx \frac{\partial_x}{e^{\partial_x} - 1} F(x) = \int_0^\infty dx \sum_{k=0}^\infty B_k \frac{\partial_x^k}{k!} F(x).$$
(117)

The l.h.s. of Eq. (117) is then

$$\int_{0}^{\infty} \sum_{k=0}^{\infty} B_{k} \frac{\partial_{x}^{k}}{k!} F(x) = \int_{0}^{\infty} F(x) dx + \sum_{k=1}^{\infty} B_{k} \left[ \frac{\partial_{x}^{k-1}}{k!} F(x) \right]_{0}^{\infty}$$
$$= \int_{0}^{\infty} F(x) dx - \sum_{k=0}^{\infty} B_{k} \frac{1}{k!} F^{(k-1)}(0)$$
$$= \int_{0}^{\infty} F(x) dx + \frac{1}{2} F(0) - \sum_{k=1}^{\infty} B_{2k} \frac{1}{(2k)!} F^{(2k-1)}(0). \quad (118)$$

On the other hand, the r.h.s. of Eq. (117) is

$$\int_0^\infty dx \frac{\partial_x}{e^{\partial_x} - 1} F(x). \tag{119}$$

By Taylor expanding the denominator,

$$\frac{\partial_x}{e^{\partial_x} - 1} F(x) = -\sum_{n=0}^{\infty} \partial_x e^{n\partial_x} F(x).$$
(120)

Note that  $e^{a\partial_x}F(x) = \sum_{m=0}^{\infty} \frac{1}{m!} a^m F^{(m)}(0) = F(x+a)$  and hence the r.h.s. is

$$\int_0^\infty dx \frac{\partial_x}{e^{\partial_x} - 1} F(x) = -\int_0^\infty dx \partial_x \sum_{n=0}^\infty F(x+n) = \sum_{n=0}^\infty F(n).$$
(121)

By comparing both sides of Eq. (117), we now find

$$\sum_{n=0}^{\infty} F(n) = \int_0^{\infty} F(x)dx + \frac{1}{2}F(0) - \sum_{k=1}^{\infty} B_{2k} \frac{1}{(2k)!} F^{(2k-1)}(0).$$
(122)

Moving first two terms in the r.h.s. to the l.h.s, we obtain the Euler–McLaurin formula

$$\frac{1}{2}F(0) + \sum_{n=1}^{\infty} F(n) - \int_0^{\infty} F(x)dx = -\sum_{k=1}^{\infty} B_{2k} \frac{1}{(2k)!} F^{(2k-1)}(0).$$
(123)

Wondering why all odd  $B_k$  vanish except for  $B_1$ ? It is easy to check that

$$\frac{x}{e^x - 1} + \frac{1}{2}x = \frac{x(2 + e^x - 1)}{2(e^x - 1)} = \frac{x}{2} \coth \frac{x}{2}$$
(124)

which is manifestly an even function of x.

Going back to the definition of our function F(n) Eq. (112), we find

$$F'(n) = -2n^2 f(\pi cn/d).$$
 (125)

As we will see below, we have d of order micron in our mind. This distance is far larger than the interatomic spacing, and hence  $f(\pi cn/d)$  is constant f = 1 in the region of our interest. Therefore, we can ignore derivatives  $f^{(n)}(0)$ , and hence the only important term in the Euler-McLaurin formula Eq. (114) is F'''(0) = -4. We obtain

$$U(d) - U_0(d) = -\frac{\pi^2 L^2 \hbar c}{4d^3} F'''(0) \frac{1}{4!} B_4 = -\frac{\pi^2 L^2 \hbar c}{720d^3}.$$
 (126)

In other words, there is an *attractive* force between two conducting plates

$$F = [U(d) - U_0(d)]' = \frac{\pi^2 L^2 \hbar c}{240d^4}$$
(127)

which is numerically

$$\frac{0.013 \text{dyn/cm}^2}{(d/\mu \text{m})^3}$$
(128)

per unit area. This is indeed a tiny force, but Sparnay has observed it for the first time in 1958. He placed chromium steel and aluminum plates at distances between  $0.3-2\mu$ m, attached to a spring. The plates are also connected to a capacitor. By measuring the capacitance, he could determine the distance, while the known sping constant can convert it to the force.

## 6 Matter Field

So far we used a single-particle Hamiltonian for matter (electron) and the field-theory Hamiltonian for the photons. One can of course extend the formalism by studying multi-particle Hamiltonian for matter particles, too. That is certainly required, for instance, in the study of multi-electron atoms or nuclei, where the quantum mechanical state is a product of multi-particle wave function for matter particles and a Fock state for photons.

An alternative formulation is to use the Schödinger field to describe the matter particles. Such a formulation is required especially when there is a condensate. Let us study the coupling of the Schrödinger field to the radiation field.

The action of the system is

$$S = \int dt d\vec{x} \left[ \psi^{\dagger} i\hbar \dot{\psi} + \psi^{\dagger} \frac{(\vec{\nabla} + iQ\frac{e}{c}\vec{A})^{2}}{2m} \psi + \frac{1}{8\pi} (\vec{E}^{2} - \vec{B}^{2}) \right] \\ - \frac{1}{2} \int dt d\vec{x} d\vec{y} \psi^{\dagger}(\vec{x}) \psi^{\dagger}(\vec{y}) V(\vec{x} - \vec{y}) \psi(\vec{y}) \psi(\vec{x}).$$
(129)

Here, V describes the self-interaction of the matter field. The electric charge of the Schrödinger field is Qe. In particular, the Coulomb potential among matter particles is included in the potential,  $V(\vec{x}-\vec{y}) \ni \frac{Q^2 e^2}{|\vec{x}-\vec{y}|}$ . This is because we had solved for the scalar potential  $A^0 = \phi$  explicitly in Eq. (7).

A particular interest is when the Schrödinger field acquires a condensate,  $\psi \neq 0$ . When we studied it before, we discussed Bose–Einstein condensate for a neutral particle, such as neutral atoms. This time we consider a condensate of a charged particle. It turns out this case describes superconductivity. More specifically, we discussed that a pair-wise condesate is possible for fermions, and the pair of electrons (Cooper pairs) can be described by a Schrödinger field of charge Qe = -2e.

Cooper pairs are bound because of the exchange of phonons. In other words, an electron causes distortion of the lattice by attracting positive ions around it, so that the surrounding area has net positive charge density. An electron elsewhere then sees the positive charge density and gets attracted to it. In the language of quantum field theory, it is equivalent to the effect of the phonon field causing attraction between two electrons. The fact that the phonons are responsible for binding Cooper pairs (in s-wave) was demonstrated by studying chemically-equivalent material with different isotopes. It is not understood, however, what mechanism is responsible for the binding of Cooper pairs (in d-wave!) in high- $T_c$  superconductors. I also learned from Seamus Davis that there are systems with p-wave binding, including liquid <sup>3</sup>He and some superconductors with "heavy fermions."

When  $\psi = \sqrt{\rho}$ , where  $\rho$  is the number density of the condensate, the action for the radiation field is

$$S = \int dt d\vec{x} \left[ \frac{1}{2m} \rho \left( Q \frac{e}{c} \right)^2 \vec{A}^2 + \frac{1}{8\pi} (\vec{E}^2 - \vec{B}^2) \right].$$
(130)

The Maxwell equation is then modified by the first term due to the condensate. For a static configuration  $\vec{E} = -\vec{A} = 0$ , the equation is obtained by varying the action with respect to  $\vec{A}$ ,

$$-\vec{\nabla} \times \vec{B} + 4\pi \frac{Q^2 e^2}{mc^2} \vec{A} = 0.$$
 (131)

Taking curl of the both sides,

$$\Delta \vec{B} = -4\pi \frac{Q^2 e^2}{mc^2} \vec{B}.$$
(132)

Suppose you have a constant magnetic field outside the region of the condensate (x < 0). At the boundary,  $\vec{B}$  is constant, say,  $B_z = B$ ,  $B_x = B_y = 0$ . Inside the region of the condensate (x > 0), Eq. (132) gives a solution

$$B_z(x) = B_z(0)e^{-x/\lambda_p},\tag{133}$$

where  $\lambda_p = \sqrt{mc^2/4\pi Q^2 e^2}$  is the so-called penetration length. The magnetic field is repelled out from the region of the condensate, and hence Meißner

effect. This is indeed a fascinating property of a superconductor. The magnetic field penetrates a little bit into the condensate, but not much. The magnetism is short-ranged!

Another interesting consequence of superconductivity is the quantization of magnetic flux that penetrates a superconductor. For example, consider a daughnut-shaped superconductor in the presence of a magnetic field. In this case, we cannot take  $\psi$  completely constant, but have to allow it to vary in its phase  $\psi = \sqrt{\rho} e^{i\theta(\vec{x})}$ . The potential is minimized as long as  $|\psi|^2$  is fixed (recall the discussions of Bose–Einstein condensate). Therefore the (static) field equation for the condensate field is

$$\frac{(\hbar\vec{\nabla} - i\frac{2e}{c}\vec{A})^2}{2m}\psi - V' = -\frac{(\hbar\vec{\nabla}\theta - \frac{2e}{c}\vec{A})^2}{2m}\psi = 0.$$
(134)

To satisfy this equation, the phase has to have spatial dependence

$$\hbar \vec{\nabla} \theta = \frac{2e}{c} \vec{A}.$$
(135)

In particular, when we go around the daughnut and integrate this equation along the line, we find

$$\hbar \oint \vec{\nabla}\theta \cdot d\vec{x} = \oint \frac{2e}{c} \vec{A} \cdot d\vec{x}.$$
(136)

The r.h.s. is the magnetic flux going through the daughnut using the Stokes' theorem

$$\oint \frac{2e}{c} \vec{A} \cdot d\vec{x} = \frac{2e}{c} \int (\vec{\nabla} \times \vec{A}) \cdot d\vec{S} = \frac{2e}{c} \Phi$$
(137)

while the l.h.s is

$$\hbar \oint \vec{\nabla}\theta \cdot d\vec{x} = \hbar(\theta(2\pi) - \theta(0)). \tag{138}$$

Because  $\psi$  has to be single-valued, the phase  $e^{i\theta}$  must come back to the same one as we go around the daughnut. In other words,  $\theta$  can change only by an integer multiple of  $2\pi$ . Therefore,

$$\hbar \oint \vec{\nabla} \theta \cdot d\vec{x} = 2\pi\hbar n. \tag{139}$$

Comparing both sides of the equation, we find that the magnetic flux is quantized:

$$\Phi = \frac{2\pi\hbar c}{2e}n.\tag{140}$$

Because the magnetic flux is quantized, it cannot smoothly dissipate to zero. On the other hand, the magnetic flux induces a current going around the daughnut. Then it means that the current cannot dissipate to zero, either. This is superconductivity!

The flux quantization in the unit of  $2\pi\hbar c/2e$  had an interesting application. Aharonov–Bohm effect, as discussed in 221A, had been controversial for many decades. Critics had claimed that the field strengths (electric and magnetic fields) must be the fundamental quantities in electromagnetism, because they appear in classical mechanics, but not the vector potential, which is gauge-dependent anyway. Even when experiments started showing the effect, they complained that there might be some leakage of magnetic field which had affected the electron directly. C.N. Yang suggested to shield the magnetic field by a superconductor. Then the magnetic flux is quantized in the unit of  $2\pi\hbar c/2e$ . On the other hand, the Aharonov–Bohm effect for an electron is the interference phase by  $e^{ie\Phi/\hbar c}$ . Because the Cooper pair has charge 2e, the quantized magnetic flux still allows a non-trivial interference by  $e^{ie(2\pi\hbar c/2e)/\hbar c} = -1$ . This was demonstrated by a beautiful electron holography experiment by Tonomura, which basically shut up all criticisms.

An interesting generalization of the short-ranged magnetism in superconductors appears in particle physics. Weak interaction, responsible for nuclear  $\beta$ -decay and the basic fusion process in the Sun  $pp \to d\nu_e e^+$ , are short-ranged. Its range is only  $10^{-16}$  cm, a thousandth of the size of a nucleus! But extensive experimental studies had shown that the carrier of the weak interaction, W and Z bosons, are basically the same kind of particles as the photon, which mediates a long-ranged electromagnetic interaction. How is that possible? The only possible explanation is that our whole Universe is "superconducting," making the weak interaction short-ranged in the exactly the same way that the Cooper-pair condensate makes the magnetism shortranged. The problem here is that we don't know what is condensed in our Universe. The official name for the condensate in particle physics is "Higgs boson." An intensive search for the Higgs boson had been carried out at an electron-positron collider called LEP in Geneva, Switzerland, and it yielded 2.9 sigma signal, which is not conclusive. New experiments at Tevatron, Fermilab, Illinois, starting 2001, will continue the search.