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Time-dependent perturbation theory

$$1 \rightsquigarrow 2 \rightsquigarrow 1$$

$$1 \rightsquigarrow 2 \rightarrow 1 \rightarrow 2 \rightarrow 1 \rightarrow 2 \rightsquigarrow 1$$

$$0 \rightarrow 1 \rightsquigarrow 2 \rightarrow 0 \rightarrow 2 \rightarrow 0 \rightarrow 2 \rightsquigarrow 1 \rightarrow 0$$

The interaction picture

Suppose that the Hamiltonian $H = H_0 + H_1$, where H_0 is time-independent and H_1 is time-dependent. Suppose that we prepare or measure the system such that it's in an eigenstate of H_0 , namely $H_0\psi_i = E_i\psi_i$. After some time t, due to the influence of H_1 , the initial state ψ_i will generally evolve to a superposition of eigenstates of H_0 , and the transition probability to the state ψ_j is

$$p_{i\to j} = |\langle \psi_j | e^{-iHt} | \psi_i \rangle|^2$$

and we have $\sum_{j} p_{i \to j} = 1$ due to the completeness of the eigenstates $|\psi_{j}\rangle$.

Notice that Hamiltonian at different times generally do not commute, and in that case the operator e^{-iHt} should really mean the time-ordered version of it. What we shall derive in the following should be true in the general case.

We would like to calculate the effect of H_1 on the transition probabilities $\{p_{i\rightarrow j}\}$ perturbatively – in terms of a series in H_1 . If we have $H_1=0$, then $p_{i\rightarrow j}=\delta_{ij}$. A method called the "interaction picture" simplifies the calculation somewhat. In effect, it does the following:

$$p_{i \rightarrow j} = |\langle \psi_j | e^{-iHt} | \psi_i \rangle|^2 = |\langle \psi_j | e^{iH_0t} e^{-iHt} | \psi_i \rangle|^2$$

and the unitary operator $e^{iH_0t}e^{-iHt}$ satisfies the following differential equation

$$\begin{aligned} d_t e^{iH_0 t} e^{-iHt} &= -i e^{iH_0 t} H_1 e^{-iHt} \\ &= -i e^{iH_0 t} H_1 e^{-iH_0 t} e^{iH_0 t} e^{-iHt} \\ &= : -i H_{1I} e^{iH_0 t} e^{-iHt} \end{aligned}$$

with solution given by the Dyson series

$$e^{iH_0t}e^{-iHt} = 1 - i\int_0^t dt' H_{1I} - \int_0^t dt' \int_0^{t'} dt'' H_{1I} H_{1I} + \cdots$$

and thus to first order in H_1 , the transition amplitude (up to a phase) is

$$\langle \psi_{j} | e^{iH_{0}t} e^{-iHt} | \psi_{i} \rangle = \delta_{ij} - i \int_{0}^{t} dt' \langle \psi_{j} | H_{1I} | \psi_{i} \rangle$$
$$= \delta_{ij} - i \int_{0}^{t} dt' e^{-i\omega_{ij}t'} \langle \psi_{j} | H_{1} | \psi_{i} \rangle$$

The unitary operator $e^{iH_0t}e^{-iHt}$ can also be written as

$$e^{iH_0t}e^{-iHt} = \Im\exp\left(-i\int_0^t dt' H_{1I}\right)$$

which may be generalized to

$$U_{21} := e^{iH_0t_2}e^{-iHt_{21}}e^{-iH_0t_1} = \Im\exp\left(-i\int_{t_1}^{t_2}dt'H_{1I}\right)$$

Case I: Constant perturbation

Suppose that $H_1 = V$ is a constant operator, then the transition amplitude above evaluates to

$$\langle \psi_j | e^{iH_0t} e^{-iHt} | \psi_i \rangle = \delta_{ij} + V_{ji} \frac{e^{-i\omega_{ij}t} - 1}{\omega_{ij}}$$

and if $j \neq i$, the transition probability is

$$p_{i \to j} = |V_{ji}|^2 \left(\frac{\sin \omega_{ij} t/2}{\omega_{ij}/2}\right)^2$$

which takes the form of the familiar "sinc" function. Interestingly, when t is very large, the transition probability $p_{i\rightarrow j}$ has the limiting behavior

$$\lim_{t\to\infty} p_{i\to j} = |V_{ji}|^2 2\pi t \delta^1(\omega_{ij})$$

This is a first sign of Fermi's golden rule.

However, the result above should only hold for sufficiently small t, since the expression for the transition probability does not always satisfy $p_{i \to j} \le 1$. For example,

$$\omega_{ij} = 0 \Rightarrow p_{i \to j} = |V_{ji}|^2 t^2$$

and thus we require that $t \ll |V_{ji}|^{-1}$.

Case II: Monochromatic perturbation

Suppose that $H_1 = Ve^{-i\omega t} + V^{\dagger}e^{i\omega t}$, where V is a constant operator, then the transition amplitude is equal to

$$\langle \psi_j | e^{iH_0t} e^{-iHt} | \psi_i \rangle = \delta_{ij} + V_{ji} \frac{e^{-i\omega_{ij}t} e^{-i\omega t} - 1}{\omega_{ij} + \omega} + V_{ij*} \frac{e^{-i\omega_{ij}t} e^{i\omega t} - 1}{\omega_{ij} - \omega}$$

which contains two terms if $j \neq i$, thus $p_{i \rightarrow j}$ will contain four terms if $j \neq i$.

In order to make some simplification, we may attempt to take $t \to \infty$. However, as we have remarked earlier, t cannot be taken too large, otherwise perturbation theory will break down.

We may focus on the case when ω is close to ω_{ij} or $-\omega_{ij}$. If for example ω is close to ω_{ij} , then the second term dominates, and the transition probability $p_{i\to j}$ when $j\neq i$ is approximately equal to

$$p_{i \to j} \approx |V_{ij}|^2 \left(\frac{\sin \omega_{ij-} t/2}{\omega_{ij-}/2}\right)^2$$

where $\omega_{ij-} := \omega_{ij} - \omega$.

Although we may not take $t \to \infty$, when the final state lies in a spectrum continuum, it can be justified (see Tong Chen's notes) that we may take t large, such that

$$\langle \psi_i | e^{iH_0t} e^{-iHt} | \psi_i \rangle \approx \delta_{ij} - i V_{ji} 2\pi \delta^1(\omega_{ij} + \omega) - i V_{ij*} 2\pi \delta^1(\omega_{ij} - \omega)$$

which means that if $j \neq i$,

$$p_{i \rightarrow j} \approx |V_{ji}|^2 2\pi t \delta^1(\omega_{ij} + \omega) + |V_{ij}|^2 2\pi t \delta^1(\omega_{ij} - \omega)$$

since $\omega \neq 0$, the cross terms vanishes. Here we have used one of the delta functions to evaluate the other delta function integral, and obtained t.

Einstein's coefficients

$$d_t n_1 = -B_{21} \rho_{\omega} n_1 + A_{12} n_2 + B_{12} \rho_{\omega} n_2$$

$$d_t n_2 = -d_t n_1$$

and Einstein: when $d_t n_1 = d_t n_2 = 0$,

$$\frac{n_2}{n_1} = \frac{B_{21}\rho_{\omega}}{A_{12} + B_{12}\rho_{\omega}} = e^{-\beta\omega}$$

The electromagnetic field is quantized

Let us suppose that

$$H_1 = Va + V^{\dagger}a^{\dagger}$$

which gives us the transition probability

$$p_{1,n\to2,n-1} = n_{\omega} |V_{21}|^2 2\pi t \delta^1(\omega_{21} - \omega)$$

$$p_{2,n\to1,n+1} = (n_{\omega} + 1) |V_{21*}|^2 2\pi t \delta^1(\omega_{21} - \omega)$$

and thus

$$d_t n_1 \propto -n_{\omega} |V_{21}|^2 n_1 + (n_{\omega} + 1) |V_{21}|^2 n_2$$

$$d_t n_2 = -d_t n_1$$

For phonons, the energy density is

$$\frac{E}{V} = 2 \int \frac{d^3k}{(2\pi)^3} \frac{\omega}{e^{\beta\omega} - 1} = \int \frac{k^2dk}{\pi^2} \frac{\omega}{e^{\beta\omega} - 1} = \int \frac{\omega^2d\omega}{\pi^2} \frac{\omega}{e^{\beta\omega} - 1} = \int \frac{\omega^3n_\omega d\omega}{\pi^2}$$

which gives us the spectral energy density

$$\rho_{\omega} = \frac{\omega^3 n_{\omega}}{\pi^2}$$

and we read

$$B_{21} = B_{12}$$

$$A_{12} = B_{12} \frac{\omega^3}{\pi^2}$$

The family of Green's functions

Linear response theory

We have

$$0 = e^{iHt} O_S e^{-iHt}
 = e^{iHt} e^{-iH_0t} e^{iH_0t} O_S e^{-iH_0t} e^{iH_0t} e^{-iHt}
 = e^{iHt} e^{-iH_0t} O_T e^{iH_0t} e^{-iHt}$$

and we may expand $e^{iH_0t}e^{-iHt}$ to first order in H_1 , and obtain

$$\mathcal{O} = \mathcal{O}_I - i \int_0^t dt' \mathcal{O}_I H_{1I} + i \int_0^t dt' H_{1I} \mathcal{O}_I$$

which means that the linear response is characterized by the commutator

$$\mathcal{O}_I H_{1I} - H_{1I} \mathcal{O}_I$$

at different times: \mathcal{O}_I is at time t while H_{1I} is at time t', and we have $\int_0^t dt'$.

$$\begin{split} e^{iHt_2} \circlearrowleft_{2S} e^{-iHt_2} &= e^{iH_0t_2} \circlearrowleft_{2S} e^{-iH_0t_2} - i \int_0^{t_2} dt_1 e^{iH_0t_2} \circlearrowleft_{2S} e^{-iH_0t_{21}} H_{1S} e^{-iH_0t_1} \\ &+ i \int_0^{t_2} dt_1 e^{iH_0t_1} H_{1S} e^{iH_0t_{21}} \circlearrowleft_{2S} e^{-iH_0t_2} \end{split}$$

which is easily proved by breaking the unitary evolution operator e^{-iHt} into pieces and expanding. This result is very intuitive.

An example: The simple harmonic oscillator

We have the response function at zero temperature

$$D_{\beta \to \infty} = \frac{i}{2\omega} e^{-i\omega t_{21}} \Theta_{21} - \frac{i}{2\omega} e^{-i\omega t_{12}} \Theta_{21}$$

and thus the linear response is

$$\int dt_1 \left(\frac{i}{2\omega} e^{-i\omega t_{21}} \Theta_{21} - \frac{i}{2\omega} e^{-i\omega t_{12}} \Theta_{21} \right) e^{0^+ t_1} = \frac{i}{2\omega} \left(\frac{1}{i\omega} - \frac{1}{-i\omega} \right) = \frac{1}{\omega^2}$$

which is correct, since the new equilibrium position is at $\frac{\lambda}{\omega^2}$ for $H_1 = -\lambda \phi$.

The Lehmann representation

1. The real-time Green's function.

$$\begin{split} iG_{\beta} &= \Theta_{21} p_{i} \langle \psi_{i} | \phi_{2} \phi_{1} | \psi_{i} \rangle + \eta \Theta_{12} p_{i} \langle \psi_{i} | \phi_{1} \phi_{2} | \psi_{i} \rangle \\ &= \Theta_{21} p_{i} \langle \psi_{i} | \phi_{2} | \psi_{j} \rangle \langle \psi_{j} | \phi_{1} | \psi_{i} \rangle + \eta \Theta_{12} p_{i} \langle \psi_{i} | \phi_{1} | \psi_{j} \rangle \langle \psi_{j} | \phi_{2} | \psi_{i} \rangle \\ &= \Theta_{21} p_{i} e^{i E_{ij} t_{21}} (\phi_{2S})_{ij} (\phi_{1S})_{ji} + \eta \Theta_{12} p_{i} e^{i E_{ij} t_{12}} (\phi_{1S})_{ij} (\phi_{2S})_{ji} \end{split}$$

and we have

$$\widetilde{G}_{\beta} = p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{\omega + E_{ij} + i0^+} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{\omega - E_{ij} - i0^+}$$

2.a. The retarded Green's function.

$$\begin{split} iD_{\beta+} &= \Theta_{21} p_i \langle \psi_i | \phi_2 \phi_1 | \psi_i \rangle - \eta \Theta_{21} p_i \langle \psi_i | \phi_1 \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i \langle \psi_i | \phi_2 | \psi_j \rangle \langle \psi_j | \phi_1 | \psi_i \rangle - \eta \Theta_{21} p_i \langle \psi_i | \phi_1 | \psi_j \rangle \langle \psi_j | \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i e^{iE_{ij}t_{21}} (\phi_{2S})_{ij} (\phi_{1S})_{ji} - \eta \Theta_{21} p_i e^{iE_{ij}t_{12}} (\phi_{1S})_{ij} (\phi_{2S})_{ji} \end{split}$$

and we have

$$\widetilde{D}_{\beta+} = p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{\omega + E_{ij} + i0^+} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{\omega - E_{ij} + i0^+}$$

2.b. The advanced Green's function.

$$\begin{split} -iD_{\beta-} &= \Theta_{12} p_i \langle \psi_i | \phi_2 \phi_1 | \psi_i \rangle - \eta \Theta_{12} p_i \langle \psi_i | \phi_1 \phi_2 | \psi_i \rangle \\ &= \Theta_{12} p_i \langle \psi_i | \phi_2 | \psi_j \rangle \langle \psi_j | \phi_1 | \psi_i \rangle - \eta \Theta_{12} p_i \langle \psi_i | \phi_1 | \psi_j \rangle \langle \psi_j | \phi_2 | \psi_i \rangle \\ &= \Theta_{12} p_i e^{iE_{ij}t_{21}} (\phi_{2S})_{ij} (\phi_{1S})_{ji} - \eta \Theta_{12} p_i e^{iE_{ij}t_{12}} (\phi_{1S})_{ij} (\phi_{2S})_{ji} \end{split}$$

and we have

$$\widetilde{D}_{\beta-} = p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{\omega + E_{ij} - i0^+} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{\omega - E_{ij} - i0^+}$$

3. The imaginary-time Green's function.

$$\begin{split} -\mathcal{G}_{\beta} &= \Theta_{21} p_i \langle \psi_i | \phi_2 \phi_1 | \psi_i \rangle + \eta \Theta_{12} p_i \langle \psi_i | \phi_1 \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i \langle \psi_i | \phi_2 | \psi_j \rangle \langle \psi_j | \phi_1 | \psi_i \rangle + \eta \Theta_{12} p_i \langle \psi_i | \phi_1 | \psi_j \rangle \langle \psi_j | \phi_2 | \psi_i \rangle \\ &= \Theta_{21} p_i e^{E_{ij} \tau_{21}} (\phi_{2S})_{ij} (\phi_{1S})_{ji} + \eta \Theta_{12} p_i e^{E_{ij} \tau_{12}} (\phi_{1S})_{ij} (\phi_{2S})_{ji} \end{split}$$

and we have, setting $t_1 = 0$ such that the Θ_{12} term does not contribute,

$$\widetilde{\mathfrak{G}}_{\beta} = p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{i\omega_l + E_{ij}} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{i\omega_l - E_{ij}}$$

The "master" Green's function

is defined as

$$\widetilde{\mathcal{M}}_{\beta} = p_i \frac{(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{z + E_{ij}} - \eta p_i \frac{(\phi_{1S})_{ij}(\phi_{2S})_{ji}}{z - E_{ij}}$$

or equivalently,

$$\widetilde{\mathcal{M}}_{\beta} = \frac{(p_i - \eta p_j)(\phi_{2S})_{ij}(\phi_{1S})_{ji}}{z + E_{ij}}$$

For a non-interacting Hamiltonian, when $\phi_{1S} = a^{\dagger}$ and $\phi_{2S} = a$, the master Green's function takes a very simple form:

$$\widetilde{\mathcal{M}}_{\beta} = \frac{1}{z - \varepsilon}$$

which is most easily proved by taking $|\psi_i\rangle$ to be the occupation number basis.

The spectral function

is defined as

$$\widetilde{A}_{\beta} = i\widetilde{D}_{\beta+} - i\widetilde{D}_{\beta-}$$

which is equal to

$$p_i(\phi_{2S})_{ij}(\phi_{1S})_{ji} 2\pi \delta^1(\omega + E_{ij}) - \eta p_i(\phi_{1S})_{ij}(\phi_{2S})_{ji} 2\pi \delta^1(\omega - E_{ij})$$

or equivalently,

$$(p_i - \eta p_j)(\phi_{2S})_{ij}(\phi_{1S})_{ji} 2\pi \delta^1(\omega + E_{ij})$$

We have the following exact identity

$$\int \frac{d\omega}{2\pi} \, \widetilde{A}_{\beta} = 1$$

for a general Hamiltonian, when $\phi_{1S} = a^{\dagger}$ and $\phi_{2S} = a$.

The Kramers-Kronig relations

It can be easily verified that

$$\widetilde{\mathcal{M}}_{\beta} = \int \frac{d\omega}{2\pi} \frac{\widetilde{A}_{\beta}}{z - \omega}$$

thanks to the delta function. Now we have, if im z > 0,

$$\begin{split} \widetilde{\mathcal{M}}_{\beta} &= \int \frac{d\omega}{2\pi} \frac{\widetilde{A}_{\beta}}{z - \omega} \\ &= i \int \frac{d\omega}{2\pi} \frac{\widetilde{D}_{\beta +} - \widetilde{D}_{\beta -}}{z - \omega} = i \int_{C^{-}} \frac{d\omega}{2\pi} \frac{\widetilde{D}_{\beta +} - \widetilde{D}_{\beta -}}{z - \omega} = i \int_{C^{-}} \frac{d\omega}{2\pi} \frac{\widetilde{D}_{\beta +}}{z - \omega} = i \int \frac{d\omega}{2\pi} \frac{\widetilde{D}_{\beta +}}{z - \omega} \end{split}$$

which gives us

$$\begin{split} \widetilde{D}_{\beta+} &= i \int \frac{d\omega'}{2\pi} \frac{\widetilde{D}_{\beta+}}{\omega - \omega' + i0^+} \\ \Rightarrow \widetilde{D}_{\beta+} &= i \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\widetilde{D}_{\beta+}}{\omega - \omega'} \end{split}$$

or equivalently, the Kramers-Kronig relations,

$$\operatorname{re} \widetilde{D}_{\beta+} = -\mathcal{P} \int \frac{d\omega'}{\pi} \frac{\operatorname{im} \widetilde{D}_{\beta+}}{\omega - \omega'}$$
$$\operatorname{im} \widetilde{D}_{\beta+} = \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\operatorname{re} \widetilde{D}_{\beta+}}{\omega - \omega'}$$

Scattering theory

A useful calculation

$$\begin{split} -i\int_{-\infty}^t dt' \langle \psi_j | H_{1I} | \psi_i \rangle &= -i\int_{-\infty}^t dt' e^{-i\omega_{ij}t'} \langle \psi_j | H_1 | \psi_i \rangle \\ &= -i\int_{-\infty}^t dt' e^{-i\omega_{ij}t'} e^{0^+t} \langle \psi_j | H_1 | \psi_i \rangle \\ &= \frac{1}{\omega_{ij} + i0^+} e^{-i\omega_{ij}t'} e^{0^+t} \langle \psi_j | H_1 | \psi_i \rangle \\ &= \frac{1}{\omega_{ij} + i0^+} e^{-i\omega_{ij}t'} \langle \psi_j | H_1 | \psi_i \rangle \end{split}$$

The scattering S-matrix

is defined by

$$S := U_{+\infty-\infty}$$

We have, using the calculation above,

$$S_{ii} = \langle \psi_i | U_{+\infty-\infty} | \psi_i \rangle = \delta_{ii} - i T_{ii} 2\pi \delta^1(\omega_{ij})$$

The transition probability

$$p_{i\to j} = |T_{ji}|^2 2\pi t \delta^1(\omega_{ij})$$

where we have defined

$$T = V + V \frac{1}{E_i - H_0 + i0^+} V + V \frac{1}{E_i - H_0 + i0^+} V \frac{1}{E_i - H_0 + i0^+} V + \cdots$$

The Lippmann-Schwinger equation

We define

$$|\psi_{i+}\rangle := U_{0-\infty}|\psi_i\rangle$$
$$|\psi_{i-}\rangle := U_{0+\infty}|\psi_i\rangle$$

or equivalently,

$$\begin{split} &\lim_{t \to -\infty} e^{-iHt} |\psi_{i+}\rangle = \lim_{t \to -\infty} e^{-iH_0t} |\psi_i\rangle \\ &\lim_{t \to +\infty} e^{-iHt} |\psi_{i-}\rangle = \lim_{t \to +\infty} e^{-iH_0t} |\psi_i\rangle \end{split}$$

and by definition,

$$\begin{split} S_{ji} &= \langle \psi_j | U_{+\infty-\infty} | \psi_i \rangle \\ &= \langle \psi_j | U_{+\infty0} U_{0-\infty} | \psi_i \rangle \\ &= \langle \psi_{i-} | \psi_{i+} \rangle \end{split}$$

To obtain the expression of $|\psi_{i+}\rangle$, we compute using the "useful calculation",

$$\langle \psi_j | \psi_{i+} \rangle = \langle \psi_j | U_{0-\infty} | \psi_i \rangle = \langle \psi_j | \psi_i \rangle + \langle \psi_j | \frac{1}{E_i - H_0 + i0^+} T | \psi_i \rangle$$

from which we read the Lippmann-Schwinger equation

$$\begin{aligned} |\psi_{i+}\rangle &= |\psi_i\rangle + \frac{1}{E_i - H_0 + i0^+} T |\psi_i\rangle \\ &= |\psi_i\rangle + \frac{1}{E_i - H_0 + i0^+} V |\psi_{i+}\rangle \end{aligned}$$

Since by definition $H_0|\psi_i\rangle = E_i|\psi_i\rangle$, we have

$$H_0|\psi_{i+}\rangle + V|\psi_{i+}\rangle = E_i|\psi_{i+}\rangle$$

namely $|\psi_{i+}\rangle$ is an eigenstate of the total H, with the same eigenvalue E_i . Therefore, if $|\psi_i\rangle$ is a scattering eigenstate of H_0 , then $|\psi_{i+}\rangle$ is a scattering eigenstate of H.

Scattering problem in three dimensions

The scattering problem in three dimensions is a good place to show the usefulness of the Lippmann-Schwinger equation. To set up the problem, notice that the scattering eigenstates of the free Hamiltonian H_0 are the plane waves, and thus we may take the state $|\psi_i\rangle$ to be the plane wave with wave vector k_i .

We then use the Lippmann-Schwinger equation to calculate the scattering eigenstates of the total Hamiltonian

$$|\psi_{i+}\rangle = |\psi_i\rangle + \frac{1}{E_i - H_0 + i0^+} T |\psi_i\rangle$$

Now let us compute the coordinate space wave function of the scattering eigenstates, and focus on its asymptotic behavior. Noticing the following calculation,

$$\langle x|\frac{1}{E_i - H_0 + i0^+}|y\rangle = 2m \int \frac{d^3l}{(2\pi)^3} \frac{e^{il \cdot x}e^{-il \cdot y}}{k^2 - l^2 + i0^+} = -\frac{m}{2\pi} \frac{e^{ik_i\eta}}{\eta}$$

where η is the distance between x and y. In the limit $x \to \infty$, we have

$$\frac{e^{ik_i\eta}}{n} = \frac{e^{ik_ir}}{r} e^{-ik_iy \cdot \hat{x}} = \frac{e^{ik_ir}}{r} \langle \psi_j | y \rangle$$

where $|\psi_i\rangle$ is the plane wave with wave vector $k_i = k_i \hat{x}$. Thus we read

$$\langle x|\psi_{i+}\rangle = \langle x|\psi_{i}\rangle - \frac{m}{2\pi} \frac{e^{ik_{i}r}}{r} \langle \psi_{j}|T|\psi_{i}\rangle$$

which means that asymptotically, the coordinate space wave function of the scattering eigenstates of the total H is the superposition of the incoming plane wave $|\psi_i\rangle$ and an outgoing spherical wave, modulated by an angular distribution function $-\frac{m}{2\pi}T_{ji}$. Since we already know that the transition probability is proportional to $|T_{ji}|^2$, we now know that it is, equivalently, proportional to the square of the angular distribution function.

The Wigner-Eckart theorem

The statement of the Wigner-Eckart theorem is quite intuitive: if some operators T_{jm} transform like the $|jm\rangle$ states, where j is fixed, then we have

$$\langle \alpha, jm|T_{j_1m_1}|\alpha_2, j_2m_2\rangle = \langle jm|j_1m_1, j_2m_2\rangle \langle \alpha, j\|T_{j_1}\|\alpha_2, j_2\rangle$$

where $\langle \alpha, j || T_{j_1} || \alpha_2, j_2 \rangle$ is a number that does not depend on m, m_1 or m_2 .

Rotational symmetry

In the special case that the scattering potential V is rotationally invariant, the general non-perturbative analysis above can be carried out further. In this case, the total H is rotationally invariant, and thus the scattering S- and T-matrices are rotationally invariant. In other words, they are scalar operators. The Wigner-Eckart theorem:

$$\langle E, lm|S|E', l'm'\rangle = \delta_{ll'}\delta_{mm'}\langle E, l||S||E', l'\rangle$$
$$= \delta_{ll'}\delta_{mm'}\langle E, l||S||E', l\rangle$$

Since we also know that the result should be proportional to $\delta_{EE'}$, we arrive at the conclusion that the scattering *S*-matrix is diagonal in the $|E,lm\rangle$ basis, with diagonal elements depending only on E and l,

$$\langle E, lm|S|E', l'm' \rangle = \delta_{ll'}\delta_{mm'}\delta_{EE'}S_{El}$$

and due to unitarity, the diagonal element $S_{E,l}$ can only be a phase.

The *T*-matrix is also a scalar operator, and we have, considering the case E' = E,

$$\begin{split} \langle E, lm|T|E, l'm' \rangle &= \delta_{ll'} \delta_{mm'} \langle E, l \| T \| E, l' \rangle \\ &= \delta_{ll'} \delta_{mm'} \langle E, l \| T \| E, l \rangle \\ &= \delta_{ll'} \delta_{mm'} T_{E,l} \end{split}$$

Thus we conclude that

$$S_{E,l} = 1 - 2\pi i T_{E,l}$$

Spherical harmonics

$$\mathcal{D}_{\phi\theta\psi}|jm\rangle = \mathcal{D}_{\phi\theta\psi,jm'jm}|jm'\rangle$$

We have

$$\begin{split} Y_{lm,\hat{n}*} &= \langle lm|\hat{n}\rangle \\ &= \langle lm|\mathcal{D}_{\phi\theta\psi}|\hat{z}\rangle \\ &= \langle lm|\mathcal{D}_{\phi\theta\psi}|l'm'\rangle\langle l'm'|\hat{z}\rangle \\ &= \langle lm|\mathcal{D}_{\phi\theta\psi}|lm'\rangle\langle lm'|\hat{z}\rangle \\ &= \langle lm|\mathcal{D}_{\phi\theta\psi}|l0\rangle\langle l0|\hat{z}\rangle \\ &= \mathcal{D}_{\phi\theta\psi,lml0}Y_{l0,\hat{z}*} \end{split}$$

where $Y_{l0,\hat{z}}=\sqrt{\frac{2l+1}{4\pi}}$. This calculation shows that the spherical harmonics are related to the matrix representation of the rotation operators in a simple way. Notice that

$$\mathcal{D}_{\phi\theta\psi,lml0} = \mathcal{D}_{\phi\theta0,lml0}$$

We also have

$$\begin{split} \langle E, lm | p \rangle &= \langle E, lm | \mathcal{D}_{\phi\theta\psi} | p\hat{z} \rangle \\ &= \langle E, lm | \mathcal{D}_{\phi\theta\psi} | E', l'm' \rangle \langle E', l'm' | p\hat{z} \rangle \\ &= \langle E, lm | \mathcal{D}_{\phi\theta\psi} | E, lm' \rangle \langle E, lm' | p\hat{z} \rangle \\ &= \langle E, lm | \mathcal{D}_{\phi\theta\psi} | E, l0 \rangle \langle E, l0 | p\hat{z} \rangle \\ &= \mathcal{D}_{\phi\theta\psi, lml0} \langle E, l0 | p\hat{z} \rangle \end{split}$$

Quantum field theory

Gell-Mann and Low theorem

We have, using \rightsquigarrow and \rightarrow diagrams, for example,

$$\phi_3\phi_2\phi_1 = U_{03}\phi_{3I}U_{30}U_{02}\phi_{2I}U_{20}U_{01}\phi_{1I}U_{10}$$
$$= U_{03}\phi_{3I}U_{32}\phi_{2I}U_{21}\phi_{1I}U_{10}$$

where ϕ_i are time-dependent Heisenberg operators. We also have

$$U_{0-\infty}|\Omega_{0}\rangle = \lim_{t_{-} \searrow -\infty} e^{iEt_{-}} e^{-iE_{0}t_{-}} |\Omega\rangle\langle\Omega|\Omega_{0}\rangle$$
$$\langle\Omega_{0}|U_{+\infty0} = \lim_{t_{+} \searrow +\infty} e^{iE_{0}t_{+}} e^{-iEt_{+}} \langle\Omega_{0}|\Omega\rangle\langle\Omega|$$

Notice that $U_{0-\infty}$ and $U_{+\infty 0}$ are not unitary! since t_- and t_+ are not real.

$$\langle \Omega | \phi_3 \phi_2 \phi_1 | \Omega \rangle = \frac{\langle \Omega_0 | U_{+\infty3} \phi_{3I} U_{32} \phi_{2I} U_{21} \phi_{1I} U_{1-\infty} | \Omega_0 \rangle}{\langle \Omega_0 | U_{+\infty-\infty} | \Omega_0 \rangle}$$

The path-integral

We have

$$\langle \Omega | \phi_3 \phi_2 \phi_1 | \Omega \rangle = \frac{\langle \Omega_0 | U_{+\infty 0} \phi_3 \phi_2 \phi_1 U_{0-\infty} | \Omega_0 \rangle}{\langle \Omega_0 | U_{+\infty 0} U_{0-\infty} | \Omega_0 \rangle}$$

after canceling some factors,

$$\langle \Omega | \phi_3 \phi_2 \phi_1 | \Omega \rangle = \lim_{t_- \searrow -\infty} \lim_{t_+ \searrow +\infty} \frac{\langle \Omega_0 | e^{-iHt_+} \phi_3 \phi_2 \phi_1 e^{iHt_-} | \Omega_0 \rangle}{\langle \Omega_0 | e^{-iHt_+} e^{iHt_-} | \Omega_0 \rangle}$$

In fact, we have

$$\langle \Omega | \phi_3 \phi_2 \phi_1 | \Omega \rangle = \lim_{t_- \searrow -\infty} \lim_{t_+ \searrow +\infty} \frac{\langle \Omega' | e^{-iHt_+} \phi_3 \phi_2 \phi_1 e^{iHt_-} | \Omega'' \rangle}{\langle \Omega' | e^{-iHt_+} e^{iHt_-} | \Omega'' \rangle}$$

for any $|\Omega'\rangle$ and $|\Omega''\rangle$. This is because

$$\lim_{t \searrow +\infty} e^{-iHt} = \lim_{t \searrow +\infty} e^{-iEt} |\Omega\rangle\langle\Omega|$$

Second quantization

$$\Psi = \Psi^0 + \Psi^1 + \Psi^2 + \Psi^3 + \cdots$$

or more precisely,

$$\mathcal{F} = \mathcal{H}^0 \oplus \mathcal{H}^1 \oplus \mathcal{H}^2 \oplus \mathcal{H}^3 \oplus \cdots$$

We have

$$\Psi = \Psi^0 + C_i |\psi_i\rangle + C_{ij} |\psi_i\rangle |\psi_j\rangle + C_{ijk} |\psi_i\rangle |\psi_i\rangle |\psi_k\rangle + \cdots$$

and

$$\mathcal{P}_{12}\Psi = \Psi^0 + C_i |\psi_i\rangle + C_{ij} |\psi_j\rangle |\psi_i\rangle + C_{ijk} |\psi_j\rangle |\psi_i\rangle |\psi_k\rangle + \cdots$$
$$= \Psi^0 + C_i |\psi_i\rangle + C_{ii} |\psi_i\rangle |\psi_j\rangle + C_{iik} |\psi_i\rangle |\psi_i\rangle |\psi_k\rangle + \cdots$$

which means that

$$C_{ji}...=\zeta C_{ij}...$$

Therefore, we define

$$|\psi_i\psi_j\cdots\rangle = \frac{1}{\sqrt{n!}}\sum_{\mathcal{P}}\zeta_{\mathcal{P}}|\psi_{\mathcal{P}i}\rangle|\psi_{\mathcal{P}j}\rangle\cdots$$

which is a over-complete basis of the n-particle subspace \mathcal{H}^n . Notice that

$$\langle \phi_{i} \phi_{j} \cdots | \psi_{k} \psi_{l} \cdots \rangle = \frac{1}{n!} \sum_{\mathcal{P}} \sum_{\mathcal{Q}} \zeta_{\mathcal{P}} \zeta_{\mathcal{Q}} \langle \phi_{\mathcal{P}i} | \psi_{\mathcal{Q}k} \rangle \langle \phi_{\mathcal{P}j} | \psi_{\mathcal{Q}l} \rangle \cdots$$

$$= \sum_{\mathcal{P}} \zeta_{\mathcal{P}} \langle \phi_{i} | \psi_{\mathcal{P}k} \rangle \langle \phi_{j} | \psi_{\mathcal{P}l} \rangle \cdots$$

$$= \det \begin{pmatrix} \langle \phi_{i} | \psi_{k} \rangle & \langle \phi_{i} | \psi_{l} \rangle & \cdots \\ \langle \phi_{j} | \psi_{k} \rangle & \langle \phi_{j} | \psi_{l} \rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

which, in particular, means that

$$\langle \psi_i \psi_i \cdots \psi_i \psi_j \psi_j \cdots \psi_j \cdots | \psi_i \psi_i \cdots \psi_i \psi_j \psi_j \cdots \psi_j \cdots \rangle = n_i! n_j! \cdots$$

A natural complete orthonormal basis of the n-particle subspace \mathbb{H}^n is the occupation number basis

$$|\cdots n_i \cdots n_j \cdots\rangle = \frac{|\cdots \psi_i \psi_i \cdots \psi_i \cdots \psi_j \psi_j \cdots \psi_j \cdots\rangle}{\sqrt{\cdots n_i! \cdots n_j! \cdots}}$$

Creation and annihilation operators

We define

$$(a_{\psi})^{\dagger}|\psi_{i}\psi_{j}\cdots\rangle:=|\psi\psi_{i}\psi_{j}\cdots\rangle$$

such that using

$$\langle \phi_i \phi_j \cdots | a_{\psi} | \psi_k \psi_l \cdots \rangle = \langle \psi_k \psi_l \cdots | (a_{\psi})^{\dagger} | \phi_i \phi_j \cdots \rangle^*$$

$$= \langle \psi_k \psi_l \cdots | \psi \phi_i \phi_j \cdots \rangle^*$$

$$= \langle \psi \phi_i \phi_j \cdots | \psi_k \psi_l \cdots \rangle$$

one can prove that

$$(a_{\phi})^{\dagger}(a_{\psi})^{\dagger} - \zeta(a_{\psi})^{\dagger}(a_{\phi})^{\dagger} = 0$$

as well as

$$a_{\phi}(a_{\psi})^{\dagger} - \zeta(a_{\psi})^{\dagger} a_{\phi} = \langle \phi | \psi \rangle$$

Second quantized operators

In the Fock space, one-body operators take the form

$$\widetilde{\mathfrak{O}}_1 = \widetilde{\mathfrak{O}}_1|_{\mathcal{H}0} \oplus \widetilde{\mathfrak{O}}_1|_{\mathcal{H}1} \oplus \widetilde{\mathfrak{O}}_1|_{\mathcal{H}2} \oplus \widetilde{\mathfrak{O}}_1|_{\mathcal{H}3} \oplus \cdots$$

where $\widetilde{\mathfrak{O}}_1|_{\mathfrak{R}n}$ is like the total angular momentum of n particles

$$\widetilde{\mathcal{O}}_1|_{\mathfrak{R}_n} = (\mathcal{O}_1 \otimes 1 \otimes \cdots \otimes 1) + (1 \otimes \mathcal{O}_1 \otimes \cdots \otimes 1) + \cdots + (1 \otimes 1 \otimes \cdots \otimes \mathcal{O}_1)$$

It is easy to verify that

$$\begin{split} \widetilde{\mathcal{O}}_1 &= \mathcal{O}_{1i} (a_{\psi i})^{\dagger} a_{\psi i} \\ &= \mathcal{O}_{1i} \langle \phi_j | \psi_i \rangle \langle \psi_i | \phi_k \rangle (a_j)^{\dagger} a_k \\ &= \langle \phi_j | \mathcal{O}_1 | \phi_k \rangle (a_j)^{\dagger} a_k \end{split}$$

For two-body operators

$$\widetilde{\mathfrak{O}}_2 = \widetilde{\mathfrak{O}}_2|_{\mathcal{H}0} \oplus \widetilde{\mathfrak{O}}_2|_{\mathcal{H}1} \oplus \widetilde{\mathfrak{O}}_2|_{\mathcal{H}2} \oplus \widetilde{\mathfrak{O}}_2|_{\mathcal{H}3} \oplus \cdots$$

Notice that we may always write

$$\mathcal{O}_2 = \sum_{I \leq J} C_{IJ} \left[\left(\mathcal{O}_{1I} \otimes \mathcal{O}_{1J} \right) + \left(\mathcal{O}_{1J} \otimes \mathcal{O}_{1I} \right) \right]$$

since the two-body operator is always symmetric under permutation.

For concreteness, take \mathcal{H}^3 as an example, we have

$$\begin{split} \widetilde{\mathcal{O}}_{2}|_{\mathcal{H}3} &= C_{IJ} \left[\left(\mathcal{O}_{1I} \otimes \mathcal{O}_{1J} \otimes 1 \right) + \left(\mathcal{O}_{1I} \otimes 1 \otimes \mathcal{O}_{1J} \right) + \left(1 \otimes \mathcal{O}_{1I} \otimes \mathcal{O}_{1J} \right) \right] \\ &+ C_{IJ} \left[\left(\mathcal{O}_{1J} \otimes \mathcal{O}_{1I} \otimes 1 \right) + \left(\mathcal{O}_{1J} \otimes 1 \otimes \mathcal{O}_{1I} \right) + \left(1 \otimes \mathcal{O}_{1J} \otimes \mathcal{O}_{1I} \right) \right] \end{split}$$

where we have suppressed the $\sum_{I \leq J}$ symbol. Now this can be written as

$$\widetilde{\mathcal{O}}_2|_{\mathcal{H}_3} = C_{IJ}\widetilde{\mathcal{O}}_{1I}|_{\mathcal{H}_3}\widetilde{\mathcal{O}}_{1J}|_{\mathcal{H}_3} - C_{IJ}\widetilde{\mathcal{O}}_{1I}\widetilde{\mathcal{O}}_{1J}|_{\mathcal{H}_3}$$

where

$$\widetilde{\mathcal{O}}_{1I}\widetilde{\mathcal{O}}_{1J}|_{\mathcal{H}3} = \left(\mathcal{O}_{1I}\mathcal{O}_{1J}\otimes 1\otimes 1\right) + \left(1\otimes\mathcal{O}_{1I}\mathcal{O}_{1J}\otimes 1\right) + \left(1\otimes 1\otimes\mathcal{O}_{1I}\mathcal{O}_{1J}\right)$$

The two-particle operator can now be written as

$$\begin{split} \widetilde{\mathbb{O}}_{2} &= C_{IJ} \langle \phi_{i} | \mathbb{O}_{1I} | \phi_{j} \rangle \langle \phi_{k} | \mathbb{O}_{1J} | \phi_{l} \rangle \langle a_{i} \rangle^{\dagger} a_{j} \langle a_{k} \rangle^{\dagger} a_{l} - C_{IJ} \langle \phi_{i} | \mathbb{O}_{1I} | \phi_{l} \rangle \langle a_{i} \rangle^{\dagger} a_{l} \\ &= C_{IJ} \langle \phi_{i} | \mathbb{O}_{1I} | \phi_{j} \rangle \langle \phi_{k} | \mathbb{O}_{1J} | \phi_{l} \rangle \langle a_{i} \rangle^{\dagger} a_{j} \langle a_{k} \rangle^{\dagger} a_{l} - C_{IJ} \langle \phi_{i} | \mathbb{O}_{1I} | \phi_{j} \rangle \langle \phi_{k} | \mathbb{O}_{1J} | \phi_{l} \rangle \langle a_{i} \rangle^{\dagger} a_{l} \delta_{jk} \\ &= C_{IJ} \langle \phi_{i} | \mathbb{O}_{1I} | \phi_{j} \rangle \langle \phi_{k} | \mathbb{O}_{1J} | \phi_{l} \rangle \langle a_{i} \rangle^{\dagger} \langle a_{k} \rangle^{\dagger} a_{l} a_{j} \\ &= C_{IJ} \langle \phi_{k} | \mathbb{O}_{1J} | \phi_{l} \rangle \langle \phi_{i} | \mathbb{O}_{1J} | \phi_{i} \rangle \langle a_{k} \rangle^{\dagger} \langle a_{l} \rangle^{\dagger} a_{l} a_{l} \end{split}$$

and we finally conclude that

$$\widetilde{\mathcal{O}}_2 = \frac{1}{2} \langle \phi_i | \langle \phi_k | \mathcal{O}_2 | \phi_j \rangle | \phi_l \rangle (a_i)^{\dagger} (a_k)^{\dagger} a_l a_j$$

The number operator

is the identity operator $1:\mathcal{H}^1\to\mathcal{H}^1$ lifted to the Fock space: $\mathcal{N}=(a_j)^\dagger a_j$.

Quantum statistical mechanics

is governed by

$$\rho = Z^{-1}e^{-\beta\mathcal{H} + \beta\mu\mathcal{N}}$$

The Legendre transformation

We have

$$Z = e^{iW} = \int D\phi \, e^{iS + iJ \cdot \phi}$$

such that the expectation value

$$\phi_{\text{exp}} = \frac{1}{iZ} \frac{\partial Z}{\partial J} = \frac{\partial W}{\partial J}$$

The effective action Γ is defined by the following Legendre transformation

$$-\Gamma = I \cdot \phi - W$$

and should be viewed as a function of ϕ ,

$$-\delta\Gamma = \delta J \cdot \phi + J \cdot \delta \phi - \frac{\partial W}{\partial I} \cdot \delta J = J \cdot \delta \phi$$

The effective action

We define a path-integral using the effective action in place of the action

$$Z_{\Gamma} = \int D\phi \, e^{i\Gamma + iJ \cdot \phi}$$

We may use the saddle point approximation, which requires that

$$\frac{\partial \Gamma}{\partial \phi} + J = 0$$

and we have

$$Z_{\Gamma} \approx e^{i\Gamma + iJ\cdot\phi} = e^{iW}$$

which means that the original Z and W can be computed by drawing tree diagrams of the effective action only! We thus conclude that the propagator and interaction vertices in the expression of the effective action are **exact**.

The quantum variational principle

Finally, notice that at J = 0, we have

$$\delta\Gamma = -J \cdot \delta\phi = 0$$

and the field is now equal to

$$\frac{\partial W}{\partial I}|_{J=0} = \phi_{\exp}|_{J=0}$$

namely $\phi_{\rm exp}|_{J=0}$ is the solution to the equation $\delta\Gamma=0$. This is to be compared with the fact that $\phi_{\rm cl}$ is the solution to the equation $\delta S=0$.

Conformal transformations

A map $\phi: (M_1, g_1) \rightarrow (M_2, g_2)$ is called conformal if

$$\phi^* g_2 = \Omega^2 g_1$$

or equivalently in local coordinates,

$$g_{2\mu\nu}\frac{\partial x^{2\mu}\circ\phi}{\partial x^{1\rho}}\frac{\partial x^{2\nu}\circ\phi}{\partial x^{1\sigma}}=\Omega^2g_{1\rho\sigma}$$

Noether's theorem

For the shift $\psi' = \psi + \delta \psi$, where $\delta \psi$ may depend on ψ ,

$$\begin{split} \delta \mathcal{L} &= \frac{\partial \mathcal{L}}{\partial \psi} \delta \psi + \frac{\partial \mathcal{L}}{\partial \partial_{\mu} \psi} \delta \partial_{\mu} \psi \\ &= \partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial \partial_{\mu} \psi} \right) \delta \psi + \frac{\partial \mathcal{L}}{\partial \partial_{\mu} \psi} \partial_{\mu} \delta \psi + \frac{\partial S}{\partial \psi} \delta \psi \\ &= \partial_{\mu} \left(\frac{\partial \mathcal{L}}{\partial \partial_{\mu} \psi} \delta \psi \right) + \frac{\partial S}{\partial \psi} \delta \psi \end{split}$$

namely some current is conserved on-shell.

The Ward identity

For the shift $\phi' = \phi + \delta \phi$, where $\delta \phi$ may depend on ϕ ,

$$\int D\phi e^{-S} X = \int D\phi' e^{-S'} X'$$

$$= \int D\phi e^{-S} \left(1 - \int d^2 x \, T_{\mu\nu} \partial_{\mu} \varepsilon_{\nu} \right) (X + \delta X)$$

$$0 = \int D\phi e^{-S} \left(\delta X - X \int d^2 x \, T_{\mu\nu} \partial_{\mu} \varepsilon_{\nu} \right)$$

$$= \int D\phi e^{-S} \left(\delta X + X \int d^2 x \, \varepsilon_{\nu} \partial_{\mu} T_{\mu\nu} \right)$$

Integrating the Ward identity over a small pillbox shows that $\int dx T_{0v}$ is the generator of spacetime symmetries.

The conformal Ward identity

The right-hand-side of the equation above can actually be written as

$$0 = \int D\phi \, e^{-S} \left(\delta X + X \int_{\mathcal{B}} d^2 x \, \varepsilon_{\nu} \partial_{\mu} T_{\mu\nu} \right)$$

$$= \int D\phi \, e^{-S} \left(\delta X - X \int_{\mathcal{B}} d^2 x \, T_{\mu\nu} \partial_{\mu} \varepsilon_{\nu} + X \int_{\partial \mathcal{B}} \varepsilon_{\mu\rho} dx_{\rho} \, \varepsilon_{\nu} T_{\mu\nu} \right)$$

$$0 = \int D\phi \, e^{-S} \left(\delta' X + X \int_{\partial \mathcal{B}} \varepsilon_{\mu\rho} dx_{\rho} \, \varepsilon_{\nu} T_{\mu\nu} \right)$$

The Slavnov-Taylor identity

For the shift $\phi' = \phi + \delta \phi$, where $\delta \phi$ may depend on ϕ ,

$$\int D\phi \, e^{iS+iJ\cdot\phi} = \int D\phi' \, e^{iS'+iJ\cdot\phi'}$$

$$= \int D\phi \, e^{iS+iJ\cdot\phi'} \quad \text{postulate}$$

$$= \int D\phi \, e^{iS+iJ\cdot\phi+iJ\cdot\delta\phi}$$

from which we read the Slavnov-Taylor identity

$$0 = iJ^* \cdot \int D\phi \, e^{iS + iJ * \cdot \phi} \delta\phi \qquad \text{for all } J^*$$
$$= -i \frac{\partial \Gamma}{\partial \phi^*} \cdot \int D\phi \, e^{iS + iJ * \cdot \phi} \delta\phi \qquad \text{for all } J^* \leftrightarrow \phi^*$$

Notice that by definition of J^* we have

$$\int D\phi \, e^{iS + iJ * \cdot \phi} \phi = \phi^*$$

and thus

$$0 = \frac{\partial \Gamma}{\partial \phi^*} \cdot \int D\phi \, e^{iS + iJ * \cdot \phi} \delta \phi = \frac{\partial \Gamma}{\partial \phi^*} \cdot \delta \phi^* = \delta \Gamma$$

for $\delta \phi = A \cdot \phi + b$.

The Kondo problem

The effective Hamiltonian method

We have, since $\mathcal{P}_j \mathcal{P}_j = 1$,

$$\mathcal{P}_i H \mathcal{P}_i \mathcal{P}_i \psi = E \mathcal{P}_i \psi$$

and when $\mathcal{P}_1 + \mathcal{P}_2 = 1$,

$$H_{11}\psi_1 + H_{12}\psi_2 = E\psi_1$$

$$H_{21}\psi_1 + H_{22}\psi_2 = E\psi_2$$

The second equation can be used to solve for ψ_2 ,

$$\psi_2 = \frac{1}{E - H_{22}} H_{21} \psi_1$$

which gives us a self-consistent equation

$$\left(H_{11} + H_{12} \frac{1}{E - H_{22}} H_{21}\right) \psi_1 = E \psi_1$$

Applications to degenerate perturbation theory

To second order in the perturbation,

$$H_{\text{eff}} = E_1 1 + V_{11} + V_{12} \frac{1}{E - H_{022} - V_{22}} V_{21}$$
$$\approx E_1 1 + V_{11} + V_{12} \frac{1}{E_1 - H_{022}} V_{21}$$

AFM coupling in the Hubbard model

$$H = -t \sum_{i \neq j} (a_{is})^{\dagger} a_{js} + U \sum_{i} n_{i+} n_{i-}$$

The effective Hamiltonian is equal to

$$H_{\text{eff}} = \frac{t^2}{E - U} \sum_{i \neq j} \sum_{k \neq l} (a_{is})^{\dagger} a_{js} (a_{kr})^{\dagger} a_{lr}$$
$$= \frac{t^2}{E - U} \sum_{i \neq j} (a_{is})^{\dagger} a_{js} (a_{jr})^{\dagger} a_{ir}$$

Notice that

$$\sum_{i \neq j} S_i \cdot S_j = \frac{1}{2} \sum_{i \neq j} (a_{is})^{\dagger} (a_{jr})^{\dagger} a_{js} a_{ir} - \frac{1}{4} \sum_{i \neq j} (a_{is})^{\dagger} (a_{jr})^{\dagger} a_{jr} a_{is}$$

$$= \frac{1}{2} \sum_{i \neq j} (a_{is})^{\dagger} a_{is} - \frac{1}{2} \sum_{i \neq j} (a_{is})^{\dagger} a_{js} (a_{jr})^{\dagger} a_{ir} - \frac{1}{4} \sum_{i \neq j} (a_{is})^{\dagger} a_{is} (a_{jr})^{\dagger} a_{jr}$$

$$= \frac{1}{2} - \frac{1}{2} \sum_{i \neq j} (a_{is})^{\dagger} a_{js} (a_{jr})^{\dagger} a_{ir}$$

which means that the effective Hamiltonian contains an interaction

$$H_{\text{eff}} \approx \frac{2t^2}{U} \sum_{i \neq j} S_i \cdot S_j + \frac{t^2}{-U}$$

The Anderson impurity model

$$H = \sum_{ks} \varepsilon_k n_{ks} + \sum_{ks} V_k (a_{ks})^{\dagger} A_s + \text{h.c.} + \sum_{s} \varepsilon N_s + U N_+ N_-$$

Notice that we have

$$H_{02} = H_{20} = 0$$

The low-energy effective Hamiltonian

In the low-energy subspace, we have

$$\begin{split} H_{10} \frac{1}{E - H_{00}} H_{01} &= \sum_{ks} \sum_{lr} V_{k*} V_l (A_s)^{\dagger} a_{ks} \frac{1}{E - H_{00}} (a_{lr})^{\dagger} A_r \\ &= \sum_{ks} \sum_{lr} V_{k*} V_l (A_s)^{\dagger} a_{ks} (a_{lr})^{\dagger} A_r \frac{1}{E - H_{00} - \varepsilon_l} \\ &\approx \sum_{ks} \sum_{lr} V_{k*} V_l (A_s)^{\dagger} a_{ks} (a_{lr})^{\dagger} A_r \frac{1}{\mathcal{E} - \varepsilon_l} \end{split}$$

as well as

$$\begin{split} H_{12} \frac{1}{E - H_{22}} H_{21} &= \sum_{ks} \sum_{lr} V_k V_{l*} (a_{ks})^{\dagger} A_s \frac{1}{E - H_{22}} (A_r)^{\dagger} a_{lr} \\ &= \sum_{ks} \sum_{lr} V_k V_{l*} (a_{ks})^{\dagger} A_s (A_r)^{\dagger} a_{lr} \frac{1}{E - H_{22} + \varepsilon_l} \\ &\approx \sum_{ks} \sum_{lr} V_k V_{l*} (a_{ks})^{\dagger} A_s (A_r)^{\dagger} a_{lr} \frac{1}{-\mathcal{E} - U + \varepsilon_l} \end{split}$$

and thus

$$H_{\text{l-e}} \approx H_{11} - \sum_{ks} \sum_{lr} V_{k*} V_l \left[\frac{(A_s)^{\dagger} a_{ks} (a_{lr})^{\dagger} A_r}{-\mathcal{E} + \varepsilon_l} + \frac{(a_{lr})^{\dagger} A_r (A_s)^{\dagger} a_{ks}}{\mathcal{E} + U - \varepsilon_k} \right]$$

The Kondo model

Notice that

$$s_{lk} \cdot S = \frac{1}{2} \sum_{sr} (a_{lr})^{\dagger} (A_s)^{\dagger} A_r a_{ks} - \frac{1}{4} \sum_{sr} (a_{lr})^{\dagger} (A_s)^{\dagger} A_s a_{kr}$$
$$= \frac{1}{2} \sum_{sr} (a_{lr})^{\dagger} (A_s)^{\dagger} A_r a_{ks} - \frac{1}{4} \sum_{r} (a_{lr})^{\dagger} a_{kr}$$

we see that the low-energy effective Hamiltonian contains an interaction

$$2\sum_{kl}V_{k*}V_{l}\left[\frac{1}{-\mathcal{E}+\varepsilon_{l}}+\frac{1}{\mathcal{E}+U-\varepsilon_{k}}\right]s_{lk}\cdot S$$

which is anti-ferromagnetic near the Fermi surface.

Constraints and the Hamiltonian formalism

The transverse vector field

The Lagrangian is

$$\begin{split} -\mathcal{L} &= \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} m^2 A_{\mu} A^{\mu} \\ &= \frac{1}{2} F_{0i} F^{0i} + \frac{1}{4} F_{ij} F^{ij} + \frac{1}{2} m^2 A_0 A^0 + \frac{1}{2} m^2 A_i A^i \end{split}$$

and thus

$$\Pi_0 = \frac{\partial \mathcal{L}}{\partial \partial_0 A^0} = 0 \qquad \text{constraint}$$

$$\Pi_i = \frac{\partial \mathcal{L}}{\partial \partial_0 A^i} = F_{0i}$$

therefore the Hamiltonian is

$$\begin{split} \mathcal{H} &= \Pi_{\mu} \partial_{0} A^{\mu} - \mathcal{L} \\ &= \Pi_{0} \partial_{0} A^{0} + \Pi_{i} \partial_{0} A^{i} - \mathcal{L} \\ &= \frac{1}{2} \Pi_{i} \Pi_{i} - \Pi_{i} \partial_{i} A^{0} + \frac{1}{4} F_{ij} F^{ij} + \frac{1}{2} m^{2} A_{0} A^{0} + \frac{1}{2} m^{2} A_{i} A^{i} \\ &= \frac{1}{2} \Pi_{i} \Pi_{i} + A^{0} \partial_{i} \Pi_{i} + \frac{1}{4} F_{ij} F^{ij} + \frac{1}{2} m^{2} A_{0} A^{0} + \frac{1}{2} m^{2} A_{i} A^{i} \end{split}$$

The equations of motion

are

$$\begin{split} \partial_0 A^\mu &= \frac{\partial \mathcal{H}}{\partial \Pi_\mu} + \lambda \frac{\partial \phi}{\partial \Pi_\mu} \qquad \phi \equiv \Pi_0 \\ -\partial_0 \Pi_\mu &= \frac{\partial \mathcal{H}}{\partial A^\mu} + \lambda \frac{\partial \phi}{\partial A^\mu} \end{split}$$

or more explicitly,

$$\begin{split} \partial_0 A^0 &= \lambda \\ -\partial_0 \Pi_0 &= \partial_i \Pi_i - m^2 A^0 \\ \partial_0 A^i &= \Pi_i - \partial_i A^0 \\ -\partial_0 \Pi_i &= -\partial_i \partial_i A^i + \partial_i \partial_i A^j + m^2 A^i \end{split}$$

The massive case

The consistency condition $\partial_0 \Pi_0 = 0$ requires that

$$A^0 = m^{-2} \partial_i \Pi_i$$
 also determines λ

and the condition $\partial_0 \partial_0 \Pi_0 = 0$ requires that

$$0 = \partial_0 \partial_i \Pi_i - m^2 \partial_0 A^0 = \partial_0 \partial_i \Pi_i - \partial_0 \partial_i \Pi_i = 0$$
 automatically satisfied

Therefore, no constraints other than the above two are needed. Notice that

$$\begin{aligned} \left\{\Pi_{0x}, \Pi_{0y}\right\} &= 0\\ \left\{\partial_0 \Pi_{0x}, \partial_0 \Pi_{0y}\right\} &= 0\\ \left\{\Pi_{0x}, \partial_0 \Pi_{0y}\right\} &\neq 0 \end{aligned} \qquad -\partial_0 \Pi_0 = \partial_i \Pi_i - m^2 A^0$$

and thus the two constraints are second class.

The massless case

The consistency condition $\partial_0 \Pi_0 = 0$ requires that

$$\partial_i \Pi_i = 0$$

and the condition $\partial_0 \partial_0 \Pi_0 = 0$ requires that

$$0 = \partial_i \partial_0 \Pi_i = \partial_i \partial_j \partial_j A^i - \partial_i \partial_j \partial_i A^j = 0 \qquad \text{automatically satisfied}$$

Therefore, no constraints other than the above two are needed. Notice that

$$\begin{split} \left\{\Pi_{0x},\Pi_{0y}\right\} &= 0 \\ \left\{\partial_0\Pi_{0x},\partial_0\Pi_{0y}\right\} &= 0 \\ \left\{\Pi_{0x},\partial_0\Pi_{0y}\right\} &= 0 \end{split} \qquad -\partial_0\Pi_0 = \partial_i\Pi_i \end{split}$$

and thus the two constraints are first class.

Miscellaneous

The guiding center coordinates

are conserved, namely they commute with the Hamiltonian, and we have

$$[X, Y] = [x + l^2 \pi_y, y - l^2 \pi_x] = -i l^2$$

Notice that they travel on equipotential lines

$$i\dot{X}_1 = [X_1, V] = -il^2 \partial_2 V$$
$$i\dot{X}_2 = [X_2, V] = +il^2 \partial_1 V$$

Spin-waves and magnons

The Schwinger-boson representation

$$S_{+} = a^{\dagger}b$$

$$S_{-} = b^{\dagger}a$$

$$2S_{z} = a^{\dagger}a - b^{\dagger}b$$

gives us the Holstein-Primakoff transformation if we use the constraint

$$a^{\dagger}a + b^{\dagger}b = 2S$$

The spin-wave is obtained by, e.g., expanding around $S_z = -S$, namely setting

$$b = b^{\dagger} = \sqrt{2S - a^{\dagger}a} \approx \sqrt{2S}$$

The Bogoliubov transformation

In order to diagonalize a Hamiltonian of the form

$$\Psi_{i\dagger}A_{ij}\Psi_{j}$$

while keeping the commutation relations, we want

$$U^{\dagger}AU = \Lambda$$

where Λ is a diagonal matrix, as well as

$$C_{ij} = \left[\Psi_i, \Psi_{j\dagger} \right] = \left[U_{ik} \Phi_k, U_{jl*} \Phi_{l\dagger} \right] = U_{ik} U_{jl*} C_{kl} \Rightarrow C = UCU^{\dagger}$$

where *C* is, by assumption, a diagonal matrix. Therefore we have

$$CAU = UCU^{\dagger}AU = UC\Lambda$$

which means that U diagonalizes the matrix CA, with eigenvalues $C\Lambda$.

The Wilsonian renormalization group

1. The "effective action".

$$Z = \int D\phi_{\Lambda} \exp i S_{\Lambda} = \int D\phi_{\Lambda'} \exp i S_{\Lambda'} = \cdots$$

2. Effective field theory.

$$q_{\Lambda} = \frac{Q_{\Lambda}}{\Lambda^{\dim Q}}$$
 is meaningful

3. Renormalization group fix points.

$$\{q_{\Lambda'}\} = \{q_{\Lambda}\}$$
 up to a field rescaling

The three-plus-one decomposition

In Minkowski spacetime,

$$V^a = -V^b Z_b Z^a + W^a$$

such that W^a is a spatial vector

$$W^{a}Z_{a} = V^{a}Z_{a} + V^{b}Z_{b}Z^{a}Z_{a}$$
$$= V^{a}Z_{a} - V^{b}Z_{b}$$
$$= 0$$

Notice also that $Z^b\nabla_bZ^a$ is a spatial vector, since $Z^b\nabla_bZ^aZ_a=0$.