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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

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

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

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

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

$$H_0 = \frac{\pi^2}{2} + \frac{\omega^2 \phi^2}{2} \qquad H_1 = -\lambda \phi$$

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 $\frac{\lambda}{\omega^2}$.

The Lehmann representation

1. The real-time Green's function.

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

and we have

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

2.a. The retarded Green's function.

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

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 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

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

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

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

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

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

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.

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

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

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

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

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

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

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

where

$$\widetilde{\mathcal{O}}_{1I}\widetilde{\mathcal{O}}_{1J}|_{\mathcal{H}3} = \left(\mathcal{O}_{1I}\mathcal{O}_{1J}\otimes 1\otimes 1\right) + \left(1\otimes\mathcal{O}_{1I}\mathcal{O}_{1J}\otimes 1\right) + \left(1\otimes1\otimes\mathcal{O}_{1I}\mathcal{O}_{1J}\right)$$

The two-particle operator can now be written as

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

and we finally conclude that

$$\widetilde{\mathfrak{O}}_{2} = \frac{1}{2} \langle \phi_{i} | \langle \phi_{k} | \mathfrak{O}_{2} | \phi_{j} \rangle | \phi_{l} \rangle \langle a_{i} \rangle^{\dagger} \langle a_{k} \rangle^{\dagger} a_{l} a_{j}$$

The Legendre transformation

We have

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

such that the expectation value

$$\phi_{\rm exp} = \frac{1}{iZ} \frac{\partial Z}{\partial I} = \frac{\partial W}{\partial I}$$

The effective action Γ is defined by the following Legendre transformation

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

and should be viewed as a function of ϕ ,

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

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,

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

Noether's theorem

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

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

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 Wilsonian renormalization group

1. The "effective action".

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

2. Effective field theory.

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

3. Renormalization group fix points.

$$\{q_{\Lambda'}\}_{\zeta\phi} = \{q_{\Lambda}\}_{\phi}$$

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

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

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

We can use the second equation 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

$$H_{12} \frac{1}{E - H_{22}} H_{21} = \sum_{ks} \sum_{lr} V_k V_{l*} (a_{ks})^{\dagger} A_s \frac{1}{E - H_{22}} (A_r)^{\dagger} a_{lr}$$

$$= \sum_{ks} \sum_{lr} V_k V_{l*} (a_{ks})^{\dagger} A_s (A_r)^{\dagger} a_{lr} \frac{1}{E - H_{22} + \varepsilon_l}$$

$$\approx \sum_{ks} \sum_{lr} V_k V_{l*} (a_{ks})^{\dagger} A_s (A_r)^{\dagger} a_{lr} \frac{1}{-\mathcal{E} - U + \varepsilon_l}$$

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.

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 $C\Lambda$.