Los Alamos Computational Condensed Matter Summer School: Lecture Notes

Author: Christopher Lane

LA-UR-26-21462

First Quantization

We have seen the many-body Schrödinger Equation is given by:

$$i\hbar \frac{\partial}{\partial t} \Psi(x_1, \ldots, x_n, t) = H \Psi(x_1, \ldots, x_n, t)$$

- Contains all information of system
- must obey statistics of particles i.e. Fermion / Boson. s.t. $\Psi(x_1, x_2) = \pm \Psi(x_2, x_1)$
- must impose boundary Conditions
  e.g. - Box with periodic boundaries
  - atomic potential
  - crystal lattice, Bloch wave functions.

where

$$H = \underbrace{\sum_{i=1}^{N}}_{\text{runs over all } N \text{ particles}} \underbrace{T(x_k)}_{\text{kinetic energy}} + \frac{1}{2} \underbrace{\sum_{i \neq j = 1}^{N}}_{\text{sums over all pairs of particles once}} V(x_i, x_j)$$

- Particle number is fixed
- Cumbersome for systems of $\sim 10^{23}$ particles
- Particles are either accessed one or two at a time, but the full information of the system must be carried along
- Used in independent particle methods

Second Quantization

We will introduce an elegant way of accounting for symmetry and operators of the many-particle system.
- this approach is essential for Relativistic Quantum Mechanics.
- simplifies the description of response functions e.g. $G(r, r')$
- avoids dealing with $\Psi(\{x_i\}, t)$ directly.

* Creation and Annihilation Operators & the Occupation Representation

Recall: the Harmonic Oscillator

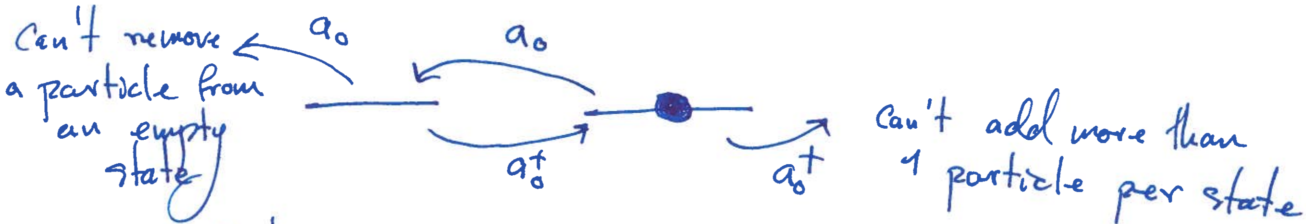
$a \equiv$ destroys one quantum excitation

$a^\dagger \equiv$ Creates one quantum excitation

We now extend this idea to particles, where operators add and remove particles from the system. Here, we will focus on the fermion case, but one can straight forwardly extend this framework to bosons.

Lets start simply. We can formally define:

$$a_0|1\rangle = |0\rangle \quad a_0|0\rangle = 0$$
$$a_0^+|0\rangle = |1\rangle \quad a_0^+|1\rangle = 0$$



From these definitions, it implies the operators obey an anticommutation relation

$$\{a_0, a_0^+\} \equiv a_0 a_0^+ + a_0^+ a_0 = 1$$

proof $(a_0 a_0^+ + a_0^+ a_0)|1\rangle = (0+1)|1\rangle = |1\rangle$
$(a_0 a_0^+ + a_0^+ a_0)|0\rangle = (1+0)|0\rangle = |0\rangle$

and $a_0^2 = 0$, $(a_0^+)^2 = 0$

can't remove 2 fermions   can't add 2 fermions

proof $a_0 a_0|1\rangle = a_0|0\rangle = 0$
$a_0^+ a_0^+|0\rangle = a_0^+|1\rangle = 0$

then the operator $N = a_0^+ a_0$ measures the number of particles in a given state:

$$N|0\rangle = a_0^+ a_0|0\rangle = 0 \;, \; N|1\rangle = a_0^+ a_0|1\rangle = 1|1\rangle$$

Now let us consider an n state system for particles to occupy. we have:

$$\{a_i, a_j^+\} = \delta_{ij} \;, \; \{a_i, a_j\} = 0 = \{a_i^+, a_j^+\} \quad i \in \text{states}$$

with $N = \sum_i a_i^+ a_i$

We can now construct the many-body occupation basis as

$$|n_0, \ldots, n_n\rangle = (a_n^\dagger)^{n_n}(a_{n-1}^\dagger)^{n_{n-1}} \cdots (a_1^\dagger)^{n_1}(a_0^\dagger)^{n_0}|0\rangle$$

Comment

There is a differance between a system of many "distinguishable particles" and many "identicle particles"

* distinguishable particles: Differance in one or more properties such as mass, charge, spin, etc...

→ If we measure the position of an electron and a positron in Coincidence [at the same time] and perform the Experimet $N \gg 1$ times, the probability that the electron is at x_n and the positron is at x_m is shown in the histogram. According to quantum mechanics the electron-positron pair collapes in the ket $|n\rangle|m\rangle$, thus the probability of finding the electron positron pair in $|n'\rangle|m'\rangle$ is zero unless $n'=n$ and $m'=m$, ie

Histogram Stefanucci & Van Leeuwen Fig 1.2

$$(\langle n'|\langle m'|)(|n\rangle|m\rangle) = \delta_{n'n}\delta_{m'm}.$$

* identicle particles: have the same internal properties such as mass, charge, spin, etc...

→ If we perform the same measurments as for the electron-positron pair, but since the particles are identicle we just use the same detector. Now if we use $|nm\rangle$ to denote a physical state in which two electrons collapse after the measurment, it is material to ask if $|nm\rangle$ & $|mn\rangle$ are two different states? However, if we only have one type of detector we can't tell the differance, thus $|mn\rangle$ is the same physical state as $|nm\rangle$.

Histogram Stefanucci & Van Leeuwen Fig 1.3

So, $|nm\rangle$ is $|mn\rangle$ up to a phase.

$$|nm\rangle = \pm |mn\rangle$$

boson (+), fermion (−)

Note: $|nm\rangle$ is Not given by nature, it is our representation that requires $|nm\rangle = e^{i\alpha}|mn\rangle$.

Now we repeat the coincidence Experiment. The probability is symmetric about $n \leftrightarrow m$, as expected, and no diagonal terms for fermions. So, the probability of finding two electrons is zero unles $n = n'$ & $m = m'$ or $n = m'$ & $m = n'$.

$$\langle n'm' | nm\rangle = \delta_{nn'}\delta_{mm'} \pm \delta_{m'n}\delta_{n'm}$$

boson (+), fermion (−)

Example: Here, the creation (annihilation) operators encode this phase in their algebra.

$$|n_0 n_1\rangle = a_1^\dagger a_0^\dagger |0\rangle = -a_0^\dagger a_1^\dagger |0\rangle = -|n_1 n_0\rangle$$

* Change of Basis *

The occupation representation can account for any labeling of the states including spin, orbital, momentum, Energy, and position. Here, we show how to construt states in any of these bases, and change between quantum numbers. In general we can expand one basis into another via the completness relation:

$$|\mu_i\rangle = \sum_m |\alpha_m\rangle\langle\alpha_m|\mu_i\rangle$$

note: $\langle\alpha_m|\alpha_n\rangle = \delta_{nm}$ orthogonality

$\sum_m |\alpha_m\rangle\langle\alpha_m| = \mathbb{1}$ completness.

This mean the creation (annihilation) operators for the two diffent bases are related by

$$c_{\mu_i}^\dagger = \sum_m a_{\alpha_m}^\dagger \underbrace{\langle\alpha_m|\mu_i\rangle}_{\text{overlap matrix elements}}$$

$$c_{\mu_i} = \sum_m a_{\alpha_m} \langle\mu_i|\alpha_m\rangle$$

if $c_{\mu_i}^\dagger$ (c_{μ_i}) obey the anticommutation relations, so does $a_{\alpha_m}^\dagger$ (a_{α_m})

Proof $\quad a_{\alpha m} a^{+}_{\alpha n} + a^{+}_{\alpha n} a_{\alpha m} = \sum_{ij} \underbrace{\left(c_{\mu_i} c^{+}_{\mu_j} + c^{+}_{\mu_j} c_{\mu_i}\right)}_{\delta_{ij}} \langle \alpha_m | \mu_i \rangle \langle \mu_j | \alpha_n \rangle$

$$= \sum_j \underbrace{\langle \alpha_m | \mu_j \rangle \langle \mu_j | \alpha_n \rangle}_{\text{Completeness} = \mathbb{1}} = \langle \alpha_m | \alpha_n \rangle = \delta_{mn}$$

In analogy, we can expand into position & momentum space

$$|\mu_i\rangle = \int d\bar{r}\ |r\rangle \underbrace{\langle r | \mu_i \rangle}_{\equiv \varphi_{\mu_i}(\bar{r}) \text{ basis functions}}$$

or in operator form

$$c^{+}_{\mu_i} = \int d\bar{r}\ \psi^{+}(\bar{r})\ \varphi_{\mu_i}(r) \quad ; \quad c_{\mu_i} = \int d\bar{r}\ \psi(r)\ \varphi^{*}_{\mu_i}(\bar{r})$$

which implies:

$$\{\psi(r), \psi^{+}(r')\} = \sum_{ij} \underbrace{\{c_{\mu_i}, c^{+}_{\mu_j}\}}_{\delta_{ij}} \varphi_{\mu_i}(r) \varphi^{*}_{\mu_j}(r') = \sum_i \varphi_{\mu_i}(r) \varphi^{*}_{\mu_i}(r') = \delta(r, r')$$

also by the same

$$\{\psi(r), \psi(r')\} = 0 = \{\psi^{+}(r), \psi^{+}(r')\}$$

Thus adding particles anticommutes with removing particles, when we happen to do the adding and removing at the same point. then the amplitude of finding the particle added at r at r' is

$$\langle r | r' \rangle = \sum_i \langle r | \mu_i \rangle \langle \mu_i | r' \rangle = \sum_i \varphi_{\mu_i}(r) \varphi^{*}_{\mu_i}(r') = \delta(r, r').$$

Using the field operators, we can construct the many-particle position basis:

$$|r_1, r_2, \dots, r_n\rangle = \psi^{+}(r_n)\, \psi^{+}(r_{n-1}) \cdots \psi^{+}(r_1) |0\rangle$$

This basis forms a convenient basis for systems of many identical particles since they intrinsically have the right symmetry due to the anticommutation relations

Example: $\quad |r_1, \dots, r_i, r_{i+1}, \dots, r_n\rangle = \psi^{+}(r_n) \cdots \psi^{+}(r_{i+1}) \psi^{+}(r_i) \cdots \psi^{+}(r_1)|0\rangle$

$$= -\psi^{+}(r_n) \cdots \psi^{+}(r_i) \psi^{+}(r_{i+1}) \cdots \psi^{+}(r_1)|0\rangle$$

$$= -|r_1 \dots r_{i+1}\, r_i \dots r_n\rangle$$

If we wish to remove a particle from the many-particle system we find:

$$\psi(x)|r_1 \cdots r_N\rangle = \sum_{k=1}^{N} (\pm)^{N+k}\,\delta(x, r_k)\,|r_1 \cdots r_{k-1} r_{k+1} \cdots r_N\rangle$$

Example:

$$\begin{aligned}\psi(x)|r_1 r_2\rangle &= \psi(x)\,\psi^{+}(r_2)\,\psi^{+}(r_1)|0\rangle \\ &= \left[\delta(x, r_2) - \psi^{+}(r_2)\,\psi(x)\right]\psi^{+}(r_1)|0\rangle \\ &= \delta(x, r_2)|r_1\rangle - \psi^{+}(r_2)\,\psi(x)\,\psi^{+}(r_1)|0\rangle \\ &= \delta(x, r_2)|r_1\rangle - \psi^{+}(r_2)\left[\delta(x, r_1) - \cancel{\psi^{+}(r_1)\,\psi(x)}^{\,0}\right]|0\rangle \\ &= \delta(x, r_2)|r_1\rangle - \delta(x, r_1)|r_2\rangle\end{aligned}$$

So, the annihilation operator removes systematically a particle from every position coordinate while keeping the result totally antisymmetric.

Note

$$\underbrace{\psi^{+}(r)|0\rangle}_{\text{acts to the right}} = \underbrace{\langle 0|\psi(r)}_{\text{acts to the left}} \quad \text{since} \quad \left[\psi^{+}(r)\right]^{+} = \psi(r)$$

Then it follows that

$$\langle r_1', \ldots, r_N' | r_1, \ldots, r_N\rangle = \sum_{P} (\pm)^{P} \prod_{j=1}^{N} \delta(r_j' - r_{P_j})$$

↑ sum over all permutations of $r_1, r_2, \ldots, r_N$ ordering with even and odd permutations yielding $(\pm)^P$

This expression is for a permanent/determinant

$$|A|_{\pm} = \sum_{P} (\pm)^{P} A_{1P_1} \cdots A_{NP_N} \; ; \; \text{where } A_{ij} = \delta(r_i - r_j)$$

Thus is also

$$\langle r_1', \ldots, r_N' | r_1, \ldots, r_N\rangle = \begin{vmatrix} \delta(r_1' - r_1) & \cdots & \delta(r_1' - r_N) \\ \vdots & & \\ \delta(r_N' - r_1) & \cdots & \delta(r_N' - r_N)\end{vmatrix}$$

also

$$\frac{1}{N!}\int d\bar{r}_1 \cdots d\bar{r}_N \, |r_1, \ldots, r_N\rangle\langle r_1, \ldots, r_N| = \mathbb{1}$$

Proof: left as an exercises.

In the many-body Schrödinger Equation we have:

$$\hat{H}|\Psi(t)\rangle = i\hbar\partial_t|\Psi(t)\rangle$$

we can project onto position space to recover the first quantized form:

$$\langle r_1,\dots,r_N|\left(\hat{H}|\Psi(t)\rangle = i\hbar\partial_t|\Psi(t)\rangle\right)$$

$$H\langle r_1,\dots,r_N|\Psi(t)\rangle = i\hbar\partial_t\langle r_1,\dots r_N|\Psi(t)\rangle$$

$$H\,\Psi(r_1,\dots,r_N,t) = i\hbar\partial_t\Psi(r_1,\dots,r_N,t)$$

we can expand this into a set of quantum numbers

$$\Psi(r_1,\dots,r_N,t) = \underbrace{\langle r_1,\dots,r_N|n_1,\dots,n_N\rangle}_{\text{Basis functions}}\underbrace{\langle n_1,\dots,n_N|\Psi(t)\rangle}_{\text{Coefficients}}$$

Since $\langle r_1,\dots,r_N|n_1,\dots,n_N\rangle = \langle 0|\psi(r_1)\psi(r_2)\cdots\psi(r_N)\,c_N^\dagger\cdots c_1^\dagger|0\rangle$

and $c_i^\dagger = \int d\bar{r}\,\psi^\dagger(r)\,\varphi_i(r)$

$$= \int dr_1'\cdots dr_N'\,\langle 0|\psi(r_1)\cdots\psi(r_N)\psi^\dagger(r_N)\cdots\psi(r_1)|0\rangle\times\varphi_1(r_1')\cdots\varphi_N(r_N')$$

$$= \int d\bar{r}_1'\cdots dr_N'\,\underbrace{\langle r_1,\dots,r_N|r_1',\dots,r_N'\rangle}_{\sum_P(\pm)^P\prod_{j=1}^{N}\delta(r_j-r_{P_j}')}\varphi_1(r_1')\cdots\varphi_N(r_N')$$

$$= \sum_P(\pm)^P\prod_{j=1}^{N}\int dr_1'\cdots dr_N'\,\delta(r_j-r_{P_j}')\,\varphi_1(r_1')\cdots\varphi_N(r_N')$$

$$= \sum_P(\pm)^P\prod_{j=1}^{N}\varphi_j(r_{P_j})$$

$$\Rightarrow\quad \Psi_{1,2,\dots,N}(r_1,r_2,\dots,r_N) = \begin{vmatrix}\varphi_1(r_1)\cdots\varphi_1(r_N)\\ \vdots\\ \varphi_N(r_1)\cdots\varphi_N(r_N)\end{vmatrix}$$

Which is a Slater determinant!

* Second Quantized Operators *

So far we have concentrated on re-expressing the many-body wave function into the occupation representation. Now we will convert 1st quantized operators to 2nd quantized representation.

Lets consider the center of mass operator

$$\hat{R}_{cm} = \frac{1}{N}\sum_{j=1}^{N} \hat{r}_j$$

Note: this is short hand notation for $\hat{R}_{cm} = \frac{1}{N}\left(\hat{r}_1 \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{N-1 \text{ units}} + \mathbb{1} \otimes \hat{r}_2 \otimes \underbrace{\cdots \otimes \mathbb{1}}_{N-2 \text{ units}} + \cdots\right)$

thus if this acts on $|r_1 r_2\rangle = \dfrac{|r_1\rangle|r_2\rangle \pm |r_2\rangle|r_1\rangle}{\sqrt{2}}$

$$R_{cm}|r_1 r_2\rangle = \frac{1}{2}(r_1+r_2)|r_1 r_2\rangle$$

alternatively we can write R_{cm} as:

$$R_{cm} = \frac{1}{N}\int d\bar{r}\, \bar{r}\left(\sum_i^N \delta(r-r_i)\right)$$

we recognize $\sum_i^N \delta(r-r_i)$ as the particle density operator in first quantized form.

we know: $\psi^\dagger(x)\psi(x)|y\rangle = \delta(x,y)|y\rangle$, so how does this generalize?

$$\longrightarrow \psi^\dagger(x)\psi(x)|y_1 y_2 \cdots y_N\rangle = \sum_i^N \delta(x-y_i)|y_1 \cdots y_N\rangle$$

so $R_{cm} = \dfrac{1}{\hat{N}}\int d\bar{r}\, \bar{r}\, \hat{n}(r) = \dfrac{1}{\hat{N}}\int d\bar{r}\, \bar{r}\, \hat{\psi}^\dagger(r)\hat{\psi}(r)$ in 2nd quantized form

Now for a general single-particle operator

$$\hat{O}|\alpha_1 \alpha_2 \cdots \alpha_N\rangle = \left(\sum_i O_{\alpha_i}\right)\underbrace{|\alpha_1 \alpha_2 \cdots \alpha_N\rangle}_{\frac{1}{\sqrt{N!}}\sum_P (-)^P |\alpha_{P_1}\rangle|\alpha_{P_2}\rangle\cdots|\alpha_{P_N}\rangle}$$

$$\hat{O} = \sum_i O_{\alpha_i} n_{\alpha_i} \xrightarrow[\text{Transformation}]{\text{Basis}} \hat{O} = \int dr \int dr'\, \psi^\dagger(r)\langle r|O|r'\rangle \psi(r')$$

Some examples:

$$\boxed{\begin{array}{l}\text{Richayzen} \\ \text{Table A.1}\end{array}}$$

2- particle operators

$$\hat{U}\,|\alpha_1\alpha_2\cdots\alpha_N\rangle = \left(\frac{1}{2}\sum_{i\neq j=1}^{N} U_{ij}\right)|\alpha_1\alpha_2\cdots\alpha_N\rangle$$

we know $n_\beta = \sum_i \delta(\beta-\alpha_i)$, so $n_\beta n_\gamma = \sum_{ij}\delta(\beta-\alpha_i)\,\delta(\gamma-\alpha_j)$
but we must have $i\neq j$, so we must remove $i=j$

$$n_\beta n_\gamma - \delta_{\beta\gamma}\, n_\beta$$

thus

$$\hat{U} = \frac{1}{2}\sum_{ij}^{N} U_{ij}\left(n_i n_j - \delta_{ij} n_i\right)$$

transforming to position space

$$\hat{U} = \frac{1}{2}\int d\bar{r}\int d\bar{r}'\; U(r,r')\Big(n(r)\,n(r') - \delta(r-r')\,n(r)\Big)$$

$$= \frac{1}{2}\int d\bar{r}\int d\bar{r}'\; U(r,r')\Big(\psi^\dagger(r)\psi(r)\,\psi^\dagger(r')\psi(r') - \delta(r-r')\,\psi^\dagger(r)\psi(r)\Big)$$

$$= \frac{1}{2}\int d\bar{r}\int d\bar{r}'\; U(r,r')\Big(\psi^\dagger(r)\left[\delta(r-r') - \psi^\dagger(r')\psi(r)\right]\psi(r') - \delta(r-r')\,\psi^\dagger(r)\psi(r)\Big)$$

cancels

$$= \frac{1}{2}\int d\bar{r}\int d\bar{r}'\; \psi^\dagger(r)\,\psi^\dagger(r')\,U(r,r')\,\psi(r')\,\psi(r)$$

in Summary:

$$\hat{H} = \int d\bar{r}\; \psi^\dagger(r)\left(\frac{-\nabla^2}{2m}\right)\psi(r) + \frac{1}{2}\int d\bar{r}\int d\bar{r}'\; \psi^\dagger(r)\,\psi^\dagger(r')\,V(r,r')\,\psi(r')\,\psi(r)$$

Physical Example: What is the amplitude for removing a particle at r' with spin s from the ground state of a Fermi gas and return to the ground state by replacing a particle with spin s at point r?

$$G_s(r-r') = \langle\Psi_0|\,\psi_s^\dagger(r)\,\psi_s(r')\,|\Psi_0\rangle$$

The ground state is characterized by all momenta filled up to p_f

$$\langle \Psi_0 | a^{\dagger}_{ps} a_{ps} | \Psi_0 \rangle = \begin{cases} 1 & |p| \le p_f \\ 0 & |p| > p_f \end{cases}$$

So $G_s(r-r') = \frac{1}{V} \sum_p e^{-ip\cdot(r-r')} n_{ps}$

$$= \int_0^{p_f} \frac{d\bar{p}}{(2\pi)^3} e^{-ip\cdot(r-r')} = \frac{1}{(2\pi)^3} \int_0^{p_f} dp\, p^2 \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} \underbrace{\int_{-1}^{1} d\cos\theta\, e^{-ip|r-r'|\cos\theta}}_{\left.\frac{e^{-ip|r-r'|\mu}}{-ip|r-r'|}\right|_{-1}^{1}}$$

we assume $r-r' \parallel \hat{z}$

$$= \frac{2\pi}{(2\pi)^3} \int_0^{p_f} dp\, p^2 \frac{-2i \sin(p|r-r'|)}{-ip|r-r'|}$$

$dx = dp\,|r-r'|$

$x = p|r-r'|$

$$= \frac{2}{(2\pi)^2} \int_0^{x_f} \frac{dx}{|r-r'|} \left(\frac{x}{|r-r'|}\right)^2 \frac{\sin(x)}{x}$$

$$= \frac{2}{(2\pi)^2} \frac{1}{|r-r'|^3} \int_0^{x_f} x \sin(x)$$

Since $\frac{d}{dx}\left(-x\cos(x)\right) = -\cos(x) + x\sin(x)$ [integration by parts]

$$= \frac{2}{(2\pi)^2} \frac{1}{|r-r'|^3} \left[\left(-x\cos(x)\right)\Big|_0^{x_f} + \int_0^{x_f} \cos(x)\,dx \right]$$

$$= \frac{2}{(2\pi)^2} \frac{p_f^3}{\underbrace{p_f^3|r-r'|^3}_{x_f^3}} \left(\sin(x_f) - x_f\cos(x_f)\right)$$

$$= \frac{2p_f^3}{(2\pi)^2} \frac{\sin(x_f) - x_f\cos(x_f)}{x_f^3}$$

Since

$$N = \underset{\text{spin}}{2} \sum_{|p|\le p_f} 1 = \frac{2V}{(2\pi)^3} \int_0^{p_f} d\bar{p} = \frac{2V}{(2\pi)^3}\left[\frac{4}{3}\pi p_f^3\right] \to p_f^3 = 3\pi^2 \frac{N}{V} = 3\pi^2 n$$

$$G_s(r-r') = \frac{3}{2} n \frac{\sin(p_f|r-r'|) - p_f|r-r'|\cos(p_f|r-r'|)}{p_f^3|r-r'|^3}$$

G. Baym Fig. 19-1

also $= \frac{3}{2} n \frac{j_1(x)}{x}$ for $x = p_f|r-r'|$ and j_1 is the first spherical Bessel function.

References

Quantum theory of Many-Particle Systems by AL Fetter & JD Walecka

Lectures on Quantum Mechanics by G. Baym

Nonequilibrium Many-Body theory of Quantum Systems by G Stefanucci & R van Leeuwen

Green's Functions and Condensed Matter by G. Rickayzen

We have now seen how we can transform the Hamiltonian & the various one- & Two-particle operators from 1st quantization to the 2nd quantized representation, along with "rotating" between various bases (eg Energy, momentum, position, etc). However all of this has been applied for a given instance in time t. To be able to go beyond simple perturbation techniques and describe the interacting many-body system, we need to address how the system evolves in time. We will find there are three equivalent "pictures" to address this issue.

Pictures

* Schrödinger *

The time evolution of the state vector is governed by the Schrödinger Equation

$$i\hbar \partial_t |\Psi_s(t)\rangle = \hat{H} |\Psi_s(t)\rangle$$

state vector

carries the time dependence of the state

either time independent or time dependent

Since $|\Psi_s\rangle$ is normalized and probability is conserved, $|\Psi\rangle$ must evolve via an Unitary transformation

$$|\Psi_s(t)\rangle = U(t,t_0) |\Psi_s(t_0)\rangle$$

$$\Rightarrow \quad i\hbar \partial_t U(t,t_0) = \hat{H} U(t,t_0) \quad , \text{ with } \underbrace{U(t_0,t_0) = I}_{\text{initial condition}}$$

The formal solution is

[See Differential Equations and Dynamical Systems by L. Perko]

$$U(t,t_0) = e^{-i\int_{t_0}^{t} \hat{H}(t')dt'}$$

or

$$U(t,t_0) = e^{-i\hat{H}(t-t_0)}$$

if $\hat{H}(t) \to \hat{H}$ is time independent

* Heisenberg *

We will now go from Schrödinger to Heisenberg pictures.
This picture greatly simplifies the analysis of correlation functions and is used throughout the literature & textbooks.
In this picture the entire dynamics is contained in the operators, with static wave functions and equivalent to those in the Schrödinger picture at some time t_a.

Since expectation values are invariant to the picture we choose where:

$$\langle \Psi_s(t)|\hat{O}|\Psi_s(t)\rangle = \underbrace{\langle \Psi_s(t)|U(t,t_a)}_{\langle \Psi_H(t_a)|}\underbrace{U^{+}(t_a,t)\hat{O}U(t,t_a)}_{\hat{O}_H(t)}\underbrace{U^{+}(t_a,t)|\Psi_s(t)\rangle}_{|\Psi_H(t_a)\rangle}$$

in general $\hat{O}$ & U do not commute $\Rightarrow$ very complicated object!

if $U^{+}(t_a,t)$ commutes with H, and $\hat{H}$ does not depend on time we can set $t_a = 0$.

So,

$$i\hbar\partial_t|\Psi_H(t)\rangle = i\hbar\left(\partial_t U^{+}(t_a,t)\right)|\Psi_s(t)\rangle + i\hbar\, U^{+}(t_a,t)\,\partial_t|\Psi_s(t)\rangle$$

since $i\hbar\partial_t|\Psi_s(t_a)\rangle = i\hbar\partial_t U(t_a,t)|\Psi_s(t_a)\rangle = H\,U(t_a,t)|\Psi_s(t)\rangle$

$$-i\hbar\partial_t U^{+}(t_a,t) = U^{+}(t_a,t)H$$

$$= \quad i\hbar\partial_t|\Psi_H(t_a)\rangle = \underbrace{\left(-U^{+}(t_a,t)H + U^{+}(t_a,t)H\right)}_{=0}|\Psi_s(t)\rangle$$

and how do the operators evolve?

$$i\hbar \partial_t \hat{O}_H(t) = i\hbar \left(\partial_t U^\dagger(t_a,t)\right)\hat{O}\,U(t,t_a) + i\hbar\, U^\dagger(t_a,t)\frac{\partial \hat{O}}{\partial t}U(t,t_a)$$
$$+ i\hbar\, U^\dagger(t_a,t)\,\hat{O}\,\partial_t U(t,t_a)$$
$$= \left[-U^\dagger(t_a,t)\mathcal{H}\right]\hat{O}\,U(t,t_a) + i\hbar\, U^\dagger(t_a,t)\partial_t\hat{O}\,U(t,t_a)$$
$$+ U^\dagger(t_a,t)\,\hat{O}\left[\mathcal{H}\,U(t,t_a)\right]$$
$$= \left[\hat{O}_H, \hat{H}_H\right] + i\hbar\left[\partial_t\hat{O}\right]_H$$

The Heisenberg Equation of motion resemble that of the classical Equation of motion with the Poisson brackets.

The Schrödinger and Heisenberg pictures are great if the problem is solvable.

* Dirac / Interaction *

For cases where we can't out right solve the problem the Dirac/interaction picture is suitable for $\hat{H} = \hat{H}_0 + \hat{V}$ and we can obtain a solution for an expansion in $\hat{V}$.

$$\hat{H} = \hat{H}_0 + \hat{V}$$

typically
* time independent
* non-interacting

typically
* V carries time dependence
* interacting

in this picture both wave function (state vector) and the Operators are time dependent.

$$\langle \Psi_S(t)|\hat{O}|\Psi_S(t)\rangle = \underbrace{\langle\Psi_S(t)|e^{-iH_0t}}_{\langle\Psi_I(t)|}\underbrace{e^{iH_0t}\hat{O}\,e^{-iH_0t}}_{O_I(t)}\underbrace{e^{iH_0t}|\Psi_S(t)\rangle}_{|\Psi_I(t)\rangle}$$

unitary transformation of Schrödinger state at t

also

$$|\Psi_I(t)\rangle = e^{iH_0t}|\Psi_S(t)\rangle = e^{iH_0t}U(t,t_0)|\Psi_S(t_0)\rangle$$
$$= e^{iH_0t}U(t,t_0)e^{-iH_0t_0}e^{+iH_0t_0}|\Psi_S(t_0)\rangle$$
$$= \underbrace{e^{iH_0t}U(t,t_0)e^{-iH_0t_0}}_{U_I(t,t_0)}|\Psi_I(t_0)\rangle$$

<u>Note:</u> $e^A e^B = e^{A+B}$ only if $[A,B]=0$, otherwise they can't be combined.

The Equation of motion is then

$$i\hbar\, \partial_t |\Psi_I(t)\rangle = i\hbar \left(\partial_t e^{iH_0 t}\right) |\Psi_S(t)\rangle + i\hbar\, e^{iH_0 t}\, \partial_t |\Psi_S(t)\rangle$$

↑ similar to SE

$$= \underbrace{\cancel{i\,i}}_{-1}\, e^{iH_0 t} H_0 |\Psi_S(t)\rangle + e^{iH_0 t} \hat{H} |\Psi_S(t)\rangle$$

$$= e^{iH_0 t} \left[\hat{H} - \hat{H}_0\right] |\Psi_S(t)\rangle$$

$$= e^{iH_0 t}\, \hat{V}\, e^{-iH_0 t}\, e^{iH_0 t} |\Psi_S(t)\rangle$$

$$= \hat{V}_I\, |\Psi_I(t)\rangle$$

and

$$i\hbar\, \partial_t \hat{O}_I(t) = i\hbar \left(\partial_t e^{iH_0 t}\right) \hat{O}\, e^{-iH_0 t} + \underbrace{i\hbar\, e^{iH_0 t}\, \partial_t \hat{O}\, e^{-iH_0 t}}_{i\hbar\, [\partial_t \hat{O}]_I}$$

$$+ i\hbar\, e^{iH_0 t}\, \hat{O}\, \partial_t e^{-iH_0 t}$$

$$= i\hbar\, e^{iH_0 t} (iH_0)\, \hat{O}\, e^{-iH_0 t} + i\hbar\, e^{iH_0 t}\, \hat{O}\, e^{-iH_0 t} (-iH_0)$$

$$= \left(\hat{H}_0 \hat{O}_I + \hat{O}_I \hat{H}_0\right) + i\hbar \left[\partial_t \hat{O}\right]_I$$

$$= \left[\hat{O}_I, \hat{H}_0\right] + i\hbar \left[\partial_t \hat{O}\right]_I$$

This is similar to Heisenberg's Equation of motion.

A complete description of the problem can be obtained from knowledge of the time evolution operator $U_I(t,t_0) = e^{iH_0 t}\, U(t,t_0)\, e^{-iH_0 t}$

$$i\hbar\, \partial_t U_I(t,t_0) = i\hbar \left(\partial_t e^{iH_0 t}\right) U(t,t_0)\, e^{-iH_0 t_0} + i\hbar\, e^{iH_0 t}\, \partial_t U(t,t_0)\, e^{-iH_0 t_0}$$

$$+ i\hbar\, e^{iH_0 t}\, U(t,t_0)\, \cancelto{0}{\partial_t e^{-iH_0 t_0}}$$

$$= i\hbar\, e^{iH_0 t} \left(\frac{iH_0}{\hbar}\right) U(t,t_0)\, e^{-iH_0 t_0} + e^{iH_0 t} \left[\hat{H}\, U(t,t_0)\right] e^{-iH_0 t_0}$$

$$= e^{iH_0 t} \underbrace{\left(\hat{H} - \hat{H}_0\right)}_{V} U(t,t_0)\, e^{-iH_0 t_0}$$

$$= V_I(t)\, U(t,t_0)$$

The formal solution can be written as an integral equation (integrate both sides)

$$i\hbar \int_{t_0}^{t} \partial_t U_I(t,t_0) = \int_{t_0}^{t} V_I(t')\, U(t',t_0)\, dt'$$

$$U(t,t_0) - \underbrace{U(t_0,t_0)}_{\text{Boundary Condition}} = \frac{-i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')\, U(t',t_0)\, dt'$$

$$U(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} \hat{V}_I(t')\, U(t',t_0)\, dt'$$

Note if U was a c number this would be a Volterra integral equation. With this spirit, we solve using picard iteration:

$$U(t,t_0) = 1 + \left(\frac{-i}{\hbar}\right)\underbrace{\int_{t_0}^{t} dt'\, V_I(t')}_{t_0 < t' < t} + \underbrace{\left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, V_I(t')\, V_I(t'')}_{t_0 < t'' < t' < t} + \dots$$

not simply the sum of products!

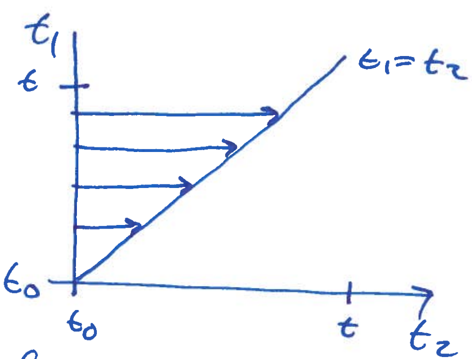
in general we have $t_0 < t^n < t^{n-1} < \dots < t' < t$.

We seemingly just made our live more complicated...

Let us examine the 2nd order term:

$$\int_{t_0}^{t} dt_1\, \hat{V}_I(t_1) \int_{t_0}^{t_1} dt_2\, \hat{V}_I(t_2)$$

$$t_0 < t_2 < t_1 < t$$



equivalently,

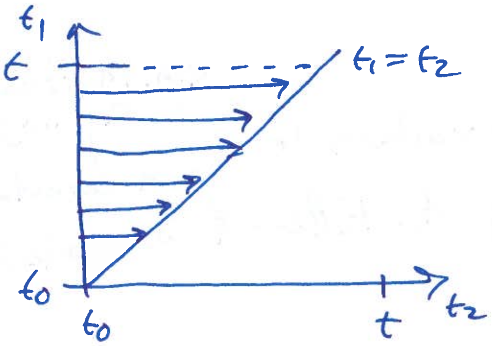
$$= \frac{1}{2}\left[\int_{t_0}^{t} dt_1\, \hat{V}_I(t_1) \int_{t_0}^{t_1} dt_2\, \hat{V}_I(t_2) + \int_{t_0}^{t} dt_1\, \hat{V}_I(t_1) \int_{t_0}^{t_1} dt_2\, \hat{V}_I(t_2)\right]$$

for a given t_1, t_2 is integrated from $t_0 \to t_1$

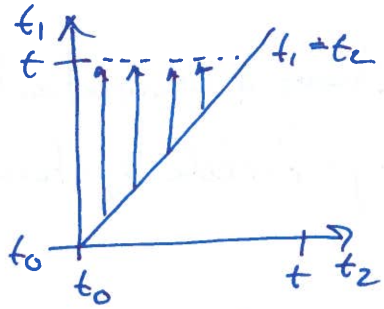
$$= \frac{1}{2}\Bigg[\underbrace{\int_{t_0}^{t} dt_1\, \hat{V}_I(t_1) \int_{t_0}^{t_1} dt_2\, \hat{V}_I(t_2)}_{\text{term \#1}} + \underbrace{\int_{t_0}^{t} dt_2\, \hat{V}_I(t_1) \int_{t_2}^{t} dt_1\, \hat{V}_I(t_1)}_{\text{term \#2}}\Bigg]$$

swap integrations

what does this mean!



term #1



term #2

for a given t_2, t_1 is integrated from $t_2 \to t$

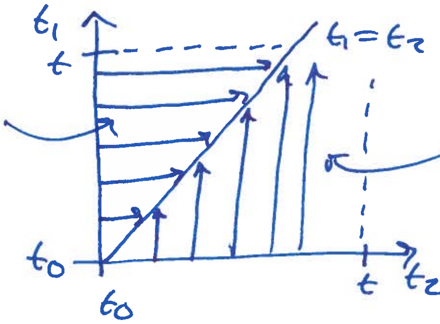
Now we change dummy indices in term #2 for $t_1 \leftrightarrow t_2$

$$= \frac{1}{2}\left[\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, \hat{V}_I(t_1)\hat{V}_I(t_2) + \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2\, \hat{V}_I(t_2)\hat{V}_I(t_1)\right]$$

we then swap integrals in term #2 again,

$$= \frac{1}{2}\left[\underbrace{\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\, \hat{V}_I(t_1)\hat{V}_I(t_2)}_{t_0 < t_2 < t_1 < t} + \underbrace{\int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1\, \hat{V}_I(t_2)\hat{V}_I(t_1)}_{t_0 < t_1 < t_2 < t}\right]$$

term #1



term #2

for a given t_2, t_1 integrates from $t_0 \to t_2$

$$= \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \left[\hat{V}_I(t_1)\hat{V}_I(t_2)\,\theta(t_1 - t_2) + \hat{V}_I(t_2)\hat{V}_I(t_2)\,\theta(t_2 - t_1)\right]$$

$$\equiv \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2\, T\left[V_I(t_1)\, V_I(t_2)\right]$$

Note: Time ordering operator was invented by Schwinger.

$$\Rightarrow \quad U(t, t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n\, T\left[V_I(t_1) \cdots V_I(t_n)\right]$$

$$\equiv T\left[e^{-i/\hbar \int_{t_0}^{t} dt' V_I(t')}\right]$$

Note: For later use,
$T[F_1(t_1)F_2(t_2)\cdots F_N(t_N)]$
$= (-1)^P F_{P_1}(t_{P_1}) \cdots F_{P_N}(t_{P_N})$

This expansion is the starting point for MBPT, S-matrix in QFT, and the Path integral.

References

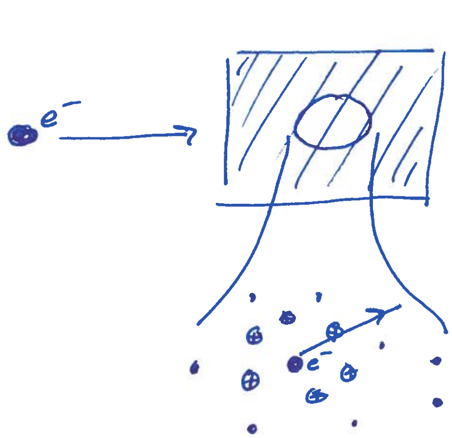
Interacting Electrons - Theory & Computational Approaches by R.M. Martin, L. Reining, & D.M. Ceperley

Quantum Theory of Many-Particle Systems by A.L. Fetter & J.D. Walecka

Green's Functions

To understand the properties of a many-body systems we typically analyze its dynamics and excitations. To accomplish this, we "probe" the system, ie perturb the system in some manner to evoke a response. The physical content of the response gives us a window into the properties of the system.

example



The many-body environment modifies the mass, charge, lifetime of the e⁻.

- charge cloud screens the charge of e⁻
- the ~~[illegible]~~ whole cloud moves with an effective mass due to the interaction between e⁻ and the many body system
- the cloud + e⁻ form a "quasiparticle"
- this quasiparticle has an effective mass, charge and life time.

Fundamental to our understanding is
how particles/excitations move through the system.

Before moving to the many-particle case, let's analyze the single particle case to determine the general relations that do not depend on the number of particles.

we know

$$|\Psi_s(t)\rangle = U(t,t_0)|\Psi_s(t_0)\rangle$$

$$\langle x|\Psi_s(t)\rangle = \int dy\, \underbrace{\langle x|U(t,t_0)|y\rangle}_{\text{"propagator"}\ \equiv\ G(xt,yt)} \langle y|\Psi_s(t_0)\rangle$$

we must have this expression obey causality

$$G(xt,yt_0) \equiv G(xt,yt_0)\,\Theta(t-t_0)$$

for $t \to t_0$ [equal time]

$$G(xt_0, yt_0) = \langle x | \underbrace{U(t_0, t_0)}_{\mathbb{1}} | y \rangle = \langle x | y \rangle = \delta(x, y)$$

The propagator is the transition amplitude of the particle between the points (y, t_0) and (x, t), and its square modulus gives the transition probability.

To gain more information on G, we have $|\Psi_s(t)\rangle$ satisfies the SE.

$$\left[i\hbar \partial_t - H(x, \partial_x, t)\right] \Psi(x,t) = 0$$

$$\Rightarrow \int dy \underbrace{\left[i\hbar \partial_t - H(x, \partial_x, t)\right] G(xt, yt_0)\, \theta(t, t_0)}_{= 0 \text{ for a general } \Psi_s(y, t_0)} \Psi_s(y, t_0) = 0$$

$$\Rightarrow \left(i\hbar \partial_t - H(x, \partial_x, t)\right) G(xt, yt_0)\, \theta(t, t_0) = 0$$

$$\left(i\hbar \partial_t - H(x, \partial_x, t)\, \theta(t, t_0)\right) G(xt, yt_0) = -i\hbar\, \delta(x, y)\, \delta(t, t_0)$$

Here, G is the Retarded Green's function of the Schrödinger Equation.

Recall

$$\hat{L} \psi = 0 \quad , \quad \hat{L} G_\psi = -\delta(x - x')$$

$\hat{L}$: Linear operator; G_ψ: Green's function

G is encoded with the boundary conditions and describe the propagation of any $\psi(y, t_0)$.

also

$$G(xt, yt_0) = \langle x | U(t, t_0) | y \rangle\, \theta(t, t_0)$$

$$= \langle 0 | \hat{\psi}(x)\, U(t, t_0)\, \hat{\psi}^\dagger(y) | 0 \rangle\, \theta(t, t_0)$$

$\langle 0|$: vacuum; $\hat{\psi}(x)$: remove the particle; $U(t, t_0)$: evolve through time; $\hat{\psi}^\dagger(y)$: add particle to the vacuum; $|0\rangle$: vacuum with this physical picture, we can define the many-body one-particle Green's function as:

$$(T_{\text{temp.}} = 0\text{K}) \qquad i\,G_{\alpha\beta}(xt, x't') = \frac{\langle \Psi_0 | T\left[\hat\psi_{H\alpha}(x,t)\,\hat\psi^\dagger_{H\beta}(x',t')\right] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

Heisenberg operators

normalization

Heisenberg ground state

$H|\Psi_0\rangle = E|\Psi_0\rangle$

$\hat\psi_{H\alpha}(x,t) = e^{i\hat H t}\,\hat\psi_\alpha(x)\,e^{-i\hat H t}$

components

i.e. spin, orbital, etc...

T is the generalized version of the time ordering operator

$$T\left[\hat\psi_{H\alpha}(x,t)\,\hat\psi^\dagger_{H\beta}(x't')\right] = \begin{cases} \hat\psi_{H\alpha}(xt)\,\hat\psi^\dagger_{H\beta}(x't') & t > t' \\ \pm\,\hat\psi^\dagger_{H\beta}(x't')\,\hat\psi_{H\alpha}(xt) & t' > t \end{cases}$$

Boson/fermion

$$iG(xt, x't') = \frac{\langle \Psi_0 | \hat\psi_{H\alpha}(xt)\,\hat\psi^\dagger_{H\beta}(x't') | \Psi_0 \rangle\,\Theta(t,t')}{\langle \Psi_0 | \Psi_0 \rangle} - \frac{\langle \Psi_0 | \hat\psi^\dagger_{H\beta}(x't')\,\hat\psi_{H\alpha}(xt) | \Psi_0 \rangle\,\Theta(t',t)}{\langle \Psi_0 | \Psi_0 \rangle}$$

* The Lehmann Representation *

assume $\langle \Psi_0 | \Psi_0 \rangle$

$$iG(xt, x't') = \langle \Psi_0 | \hat\psi_{H\alpha}(xt)\,\hat\psi^\dagger_{H\beta}(x't') | \Psi_0 \rangle\,\Theta(t,t') - \langle \Psi_0 | \hat\psi^\dagger_{H\beta}(x't')\,\hat\psi_{H\alpha}(xt) | \Psi_0 \rangle\,\Theta(t',t)$$

insert complete set of states $\qquad \sum_n |\Psi_n\rangle\langle\Psi_n| \qquad\qquad \sum_n |\Psi_n\rangle\langle\Psi_n|$

$$= \sum_n \langle \Psi_0 | e^{i\hat H t}\,\hat\psi_\alpha(x)\,e^{-i\hat H t} | \Psi_n \rangle \langle \Psi_n | e^{i\hat H t'}\,\hat\psi^\dagger_\beta(x')\,e^{-i\hat H t'} | \Psi_0 \rangle\,\Theta(t,t')$$

$$- \langle \Psi_0 | e^{i\hat H t'}\,\hat\psi^\dagger_\beta(x')\,e^{-i\hat H t'} | \Psi_n \rangle \langle \Psi_n | e^{i\hat H t}\,\hat\psi_\alpha(x)\,e^{-i\hat H t} | \Psi_0 \rangle\,\Theta(t',t)$$

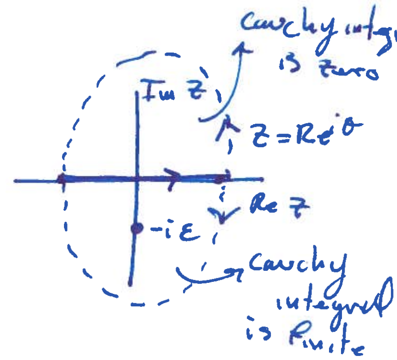
$$= \sum_n e^{iEt - iE_n t + iE_n t' - iEt'} \langle \Psi_0 | \hat\psi_\alpha(x) | \Psi_n \rangle \langle \Psi_n | \hat\psi^\dagger_\beta(x') | \Psi_0 \rangle\,\Theta(t,t')$$

$$- e^{iEt' - iE_n t' + iEt - iE_n t} \langle \Psi_0 | \hat\psi^\dagger_\beta(x') | \Psi_n \rangle \langle \Psi_n | \hat\psi_\alpha(x) | \Psi_0 \rangle\,\Theta(t',t)$$

$$= \sum_n e^{-i(E_n - E)(t-t')} \langle \Psi_0 | \hat{\psi}_\alpha(x) | \Psi_n \rangle \langle \Psi_n | \hat{\psi}^\dagger_\beta(x') | \Psi_0 \rangle \theta(t,t')$$

$$- e^{i(E_n - E)(t-t')} \langle \Psi_0 | \hat{\psi}^\dagger_\beta(x') | \Psi_n \rangle \langle \Psi_n | \hat{\psi}_\alpha(x) | \Psi_0 \rangle \theta(t',t)$$

We know $\theta(\tau) = \lim_{\varepsilon \to 0^+} -\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{\omega + i\varepsilon} e^{-i\tau\omega} d\omega$



if we extend ω to the complex plane $\omega \to z$

then $-i\tau z = -i\tau R(\cos\theta + i\sin\theta)$

$\to e^{-i\tau\cos\theta R + \tau\sin\theta R}$

if $\tau > 0 \Rightarrow \theta$ in lower half-plane

$\sim e^{-\tau|\sin\theta| R} \to 0$ as $R \to \infty$

if $\tau < 0 \Rightarrow$ in upper half-plane

$\sim e^{-|\tau|\sin\theta R} \to 0$ as $R \to \infty$

$$G(xt, x't') = \sum_n e^{-i(E_n - E)(t-t')} \langle \Psi_0 | \hat{\psi}_\alpha(x) | \Psi_n \rangle \langle \Psi_n | \hat{\psi}^\dagger_\beta(x') | \Psi_0 \rangle \left[\frac{-1}{2\pi i} \int_{-\infty}^{\infty} \frac{1}{\omega + i\varepsilon} e^{-i(t-t')\omega} d\omega \right]$$

$$- e^{i(E_n - E)(t-t')} \langle \Psi_0 | \hat{\psi}^\dagger_\beta(x') | \Psi_n \rangle \langle \Psi_n | \hat{\psi}_\alpha(x) | \Psi_0 \rangle \Bigg[\underbrace{\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-i\omega(t-t')} d\omega}{\omega - i\varepsilon}}_{\theta(-\tau)} \Bigg]$$

$$= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega \sum_n \Bigg[\frac{\langle \Psi_0 | \hat{\psi}_\alpha(x) | \Psi_n \rangle \langle \Psi_n | \hat{\psi}^\dagger_\beta(x') | \Psi_0 \rangle}{\omega + i\varepsilon} e^{-i(t-t')(\omega + E_n - E)}$$

$$+ \langle \Psi_0 | \hat{\psi}^\dagger_\beta(x') | \Psi_n \rangle \langle \Psi_n | \hat{\psi}_\alpha(x) | \Psi_0 \rangle e^{-i(t-t')(\omega + E - E_n)} \Bigg]$$

$$G(x, x', \omega') = \int_{-\infty}^{\infty} d\tau \, e^{+i\omega'\tau} G(x, x', \tau)$$

$$iG(x,x',\omega') = -\frac{1}{2\pi i}\int_{-\infty} d\omega \sum_n \Bigg[\frac{\langle\Psi_0|\hat\psi_\alpha(x)|\Psi_n\rangle\langle\Psi_n|\hat\psi^\dagger_\beta(x')|\Psi_0\rangle}{\omega+i\varepsilon} \underbrace{\int_{-\infty} d\tau\, e^{-i\tau(-\omega'+\omega+E_n-E)}}_{\substack{2\pi\delta(\omega+E_n-E-\omega') \\ \Rightarrow\ \omega=\omega'+E-E_n}}$$

$$+ \frac{\langle\Psi_0|\hat\psi^\dagger_\beta(x')|\Psi_n\rangle\langle\Psi_n|\hat\psi_\alpha(x)|\Psi_0\rangle}{\omega-i\varepsilon} \underbrace{\int_{-\infty}^{\infty} d\tau\, e^{-i\tau(-\omega'+\omega+E-E_n)}}_{\substack{2\pi\delta(\omega+E-E_n-\omega') \\ \Rightarrow\ \omega=E_n+\omega'-E}}$$

N+1 particle state, N+1 particle state, N particle state

$$= +i\sum_n \Bigg[\frac{\langle\Psi_0|\hat\psi_\alpha(x)|\Psi_n\rangle\langle\Psi_n|\hat\psi^\dagger_\beta(x')|\Psi_0\rangle}{\omega'+E-E_n+i\varepsilon}$$

N−1 particle state, N−1 particle state, N particle state

$$+ \frac{\langle\Psi_0|\hat\psi^\dagger_\beta(x')|\Psi_n\rangle\langle\Psi_n|\hat\psi_\alpha(x)|\Psi_0\rangle}{\omega'+E_n-E-i\varepsilon} \Bigg]$$

this means in the left hand term $E_n \equiv E_n(N+1)$, $E \equiv E(N)$ and in the right hand term $E_n \equiv E_n(N-1)$, $E \equiv E(N)$

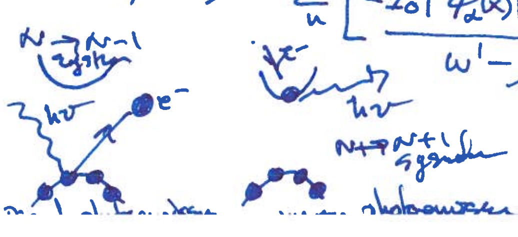
LHT

$$E - E_n = E(N) - E_n(N+1) + \big(E(N+1) - E(N+1)\big)$$
$$= -\underbrace{\big(E(N+1) - E(N)\big)}_{\substack{\text{change in the ground state} \\ \text{energy when a particle is added} \\ \text{for } N\to\infty,\ \to\mu \text{ (chemical potential)}}} - \underbrace{\big(E_n(N+1) - E(N+1)\big)}_{\substack{\text{excitation energy} \\ \text{of the } N+1 \text{ particle} \\ \text{system} \equiv \varepsilon_n(N+1)}}$$

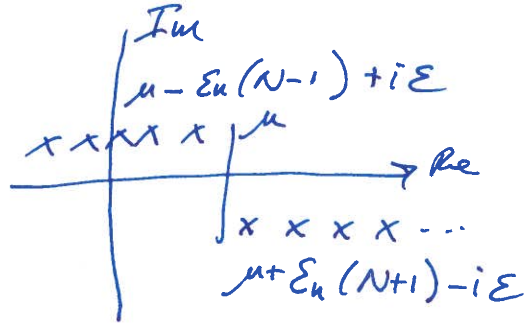
RHT

$$E_n - E \equiv E_n(N-1) - E(N) + \big(E(N-1) - E(N-1)\big)$$
$$= -\underbrace{\big(E(N) - E(N-1)\big)}_{\substack{\text{same as in the} \\ \text{LHT, } \mu \text{ in} \\ \text{the } N\to\infty \\ \text{limit}}} + \underbrace{\big(E_n(N-1) - E(N-1)\big)}_{\substack{\text{excitation energy} \\ \varepsilon_n(N-1)}}$$

$$G(x,x',\omega') = \sum_n \Bigg[\frac{\langle\Psi_0|\hat\psi_\alpha(x)|\Psi_n\rangle\langle\Psi_n|\hat\psi^\dagger_\beta(x')|\Psi_0\rangle}{\omega'-\mu-\varepsilon_n(N+1)+i\varepsilon} + \frac{\langle\Psi_0|\hat\psi^\dagger_\beta(x')|\Psi_n\rangle\langle\Psi_n|\hat\psi_\alpha(x)|\Psi_0\rangle}{\omega'-\mu+\varepsilon_n(N-1)-i\varepsilon} \Bigg]$$



This means the pole structure of $G(x,x';\omega)$ is



So G is analytic in neither the upper nor the lower ω' plane

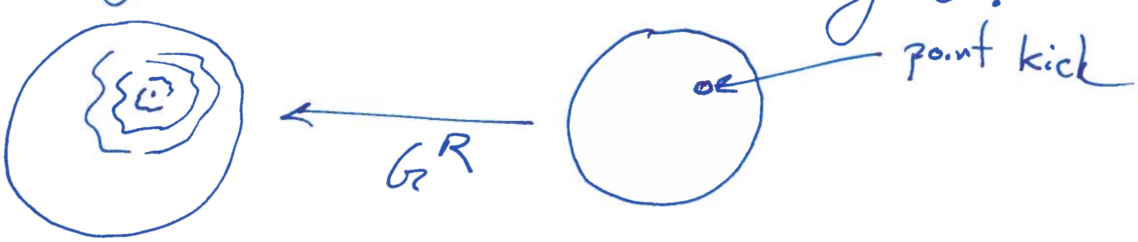
It is usefull to also define the Retarded & Advanced Green's function as

$$iG^R_{\alpha\beta}(xt,x't') = \langle\Psi_0|\{\hat\psi_{H\alpha}(xt),\hat\psi^\dagger_{H\beta}(x't')\}|\Psi_0\rangle\,\theta(t-t')$$

$$iG^A_{\alpha\beta}(xt,x't') = -\langle\Psi_0|\{\hat\psi_{H\alpha}(xt),\hat\psi^\dagger(x't')\}|\Psi_0\rangle\,\theta(t'-t)$$

anti commutator

The Retarded Green's function is usefull if we know the initial state of a system and want to know how it evolves forward in time. This is our link to Experiment and most physical quantities of interest are given in terms of G^R.



Similarly, the advanced Green's function is usefull if we know the end point configuration and we want to figure out where it came from.

The analysis of this function proceeds the same as for the time ordered Green's function. The Lehmann representation is

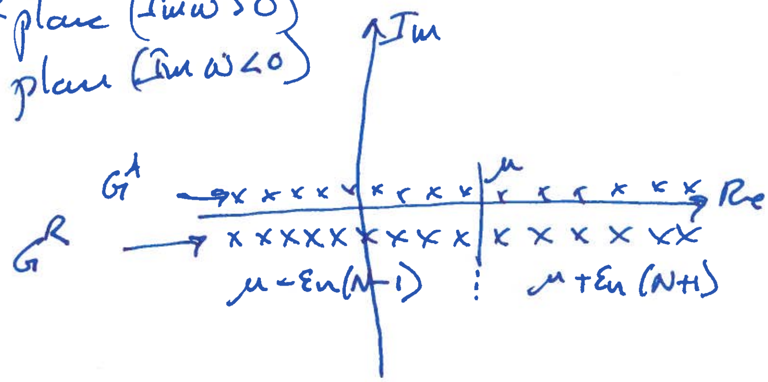
$$G^{R/A}(x,x',\omega') = \sum_n \frac{\langle \Psi_0 | \hat{\psi}_\alpha(x) | \Psi_n \rangle \langle \Psi_n | \hat{\psi}^\dagger_\beta(x') | \Psi_0 \rangle}{\omega' - \mu - E_n(N+1) \pm i\varepsilon}$$

$$+ \frac{\langle \Psi_0 | \hat{\psi}_\alpha(x) | \Psi_n \rangle \langle \Psi_n | \hat{\psi}^\dagger_\beta(x') | \Psi_0 \rangle}{\omega - \mu + E_n(N-1) \pm i\varepsilon}$$

The corresponding pole structure is

G^R analytic in ~~a~~ upper half plane ($\mathrm{Im}\,\omega > 0$)

G^A analytic in lower half plane ($\mathrm{Im}\,\omega < 0$)



For $\omega \in \mathbb{R}$

$$\left[G^R_{\alpha\beta}\right]^* = G^A_{\beta\alpha}$$

The Retarded & Advanced Green's functions differ from each other and from the Time ordered Green's function only in the convergence factors $\pm i\varepsilon$ which are important near the singularities.

~~[illegible]~~ ~~[illegible]~~ Thus, we can connect $G^{R/A}$ to G by recognizing

$$G^R_{\alpha\beta} = G_{\alpha\beta} \text{ for } \omega(\text{real}) > \mu$$

$$G^A_{\alpha\beta} = G_{\alpha\beta} \text{ for } \omega(\text{real}) < \mu$$

This brings us to the special purpose of the Time ordered Green's function. ~~Since there is not way of determining $G^{R/A}$ in an i~~ In an interacting system, we ~~[illegible]~~ can expand G in the interaction part and calculate G. Then with this we can determine $G^{R/A}$ to relate to physical problems.

we also define the spectral function as

$$A(x,x',\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G^R(x,x',\omega)$$
$$= \sum_n \langle \Psi_0 | \hat{\psi}_\alpha(x) | \psi_n\rangle\langle \psi_n | \hat{\psi}^\dagger_\beta(x') | \Psi_0\rangle\, \delta(\omega-\mu-\varepsilon_n(N+1))$$
$$+ \langle \Psi_0 | \hat{\psi}_\alpha(x) | \psi_n\rangle\langle \psi_n | \hat{\psi}^\dagger_\beta(x') | \Psi_0\rangle\, \delta(\omega-\mu+\varepsilon_n(N-1))$$

where $\int_{-\infty}^{\infty} A(x,x';\omega)\,d\omega = \delta(x-x')$

and $\int dx \int d\omega A(x\,x,\omega) = \underline{1}$ is a generalized density of states

<u>Example</u> non-interacting fermi gas.

$$g^R(k,\omega) = \frac{1}{\omega-\varepsilon_k+i\varepsilon} \Rightarrow A(k,\omega) = -\frac{1}{\pi}\mathrm{Im}\,g^R(k,\omega)$$
$$= \delta(\omega-\varepsilon_k)$$

$$g^A(k,\omega) = \frac{1}{\omega-\varepsilon_k-i\varepsilon}$$

and $\sum_k A(k,\omega) = A(\omega)$ [DOS]

$\int_{-\infty}^{\infty} A(\omega)\,d\omega = N$ electrons

$$g(k,\omega) = \frac{\theta(k-k_F)}{\omega-\varepsilon_k+i\varepsilon} + \frac{\theta(k_F-k)}{\omega-\varepsilon_k-i\varepsilon}$$

we can define

$$G(k,z) = \frac{1}{z-\varepsilon_k}$$

so that

$$g^R(k,\omega) = G(k,\omega+i\varepsilon)$$
$$g^A(k,\omega) = G(k,\omega-i\varepsilon)$$
$$g(k,\omega) = G(k,\omega+i\varepsilon\bar{f}(\omega-\varepsilon_F))$$

$$\bar{f}(\omega-\varepsilon_k) = \begin{cases} 1 & \omega > \varepsilon_F \\ -1 & \omega < \varepsilon_F \end{cases}$$

in the interacting case we will see the interacting green's function satisfying

$$G = G_0 + G_0 \Sigma G \qquad \text{Dyson's Equation}$$

where Σ is the so called self-energy and contains all the many-body physics of the problem. Thus, in the presence of interactions the spectral function is now

$$G^R(k,\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma^R(k,\omega)}$$

complex function

$$= \frac{1}{\omega - \varepsilon_k - \mathrm{Re}\,\Sigma^R(k,\omega) - i\,\mathrm{Im}\,\Sigma^R(k,\omega)}$$

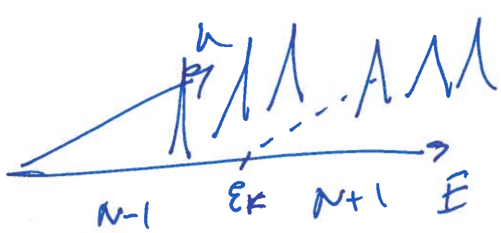
$$= \frac{\omega - \varepsilon_k - \mathrm{Re}\,\Sigma^R(k,\omega) + i\,\mathrm{Im}\,\Sigma^R(k,\omega)}{(\omega - \varepsilon_k - \mathrm{Re}\,\Sigma^R(k,\omega))^2 + (\mathrm{Im}\,\Sigma^R(k,\omega))^2}$$

$\Rightarrow$

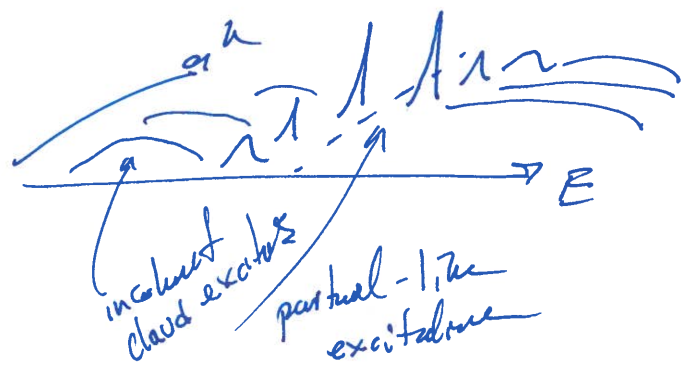
$$A(k,\omega) = -\frac{1}{\pi}\,\frac{\mathrm{Im}\,\Sigma^R(k,\omega)}{(\omega - \varepsilon_k - \mathrm{Re}\,\Sigma^R(k,\omega))^2 + (\mathrm{Im}\,\Sigma^R(k,\omega))^2}$$

if $\mathrm{Im}\,\Sigma^R(k,\omega) \to 0$

$A(k,\omega) \to \delta(\omega - \varepsilon_k - \mathrm{Re}\,\Sigma^R(k,\omega))$ for $\mathrm{Im}\,\Sigma^R(k,\omega) \neq 0$



Photoelectron spectroscopy
Stefan Hüfner
Fig 5.88



* S - Matrix *

So far we have seen that observables maybe written in terms of Green's functions and we have explored the analytic properties of the Green's functions. However all of this has been pursued within the Heisenberg picture, meaning $|\Psi\rangle$ is unknown because H is not solvable when interactions are present. In fact this is the very information we are trying to obtain from the green's function approach. To move forward, we recognize that $H = H_0 + V$, so we can use the interaction picture

$$\underset{\substack{\uparrow \\ \text{solvable}}}{H_0}$$

to recast the problem.

we know
$$|\Psi_H\rangle = \cancel{e^{}}|\Psi_S(0)\rangle = |\Psi_I(0)\rangle$$
$$= U(0,t_0)|\Psi_I(t_0)\rangle$$

so we connect $|\Psi_H\rangle$ to that in the interaction at some time before. to recover a ground state wave function we know we will introduce
$$H = H_0 + e^{-|\varepsilon| t} V$$

$\uparrow$ adiabatically switches on the interaction

therefore

$$|\Psi_H\rangle = U(0,-\infty)|\phi_0\rangle$$

where $H_0|\phi_0\rangle = \varepsilon|\phi_0\rangle$

This means we can re-write our ~~eq~~ green's function as

$$iG(xt,x't') = \frac{\langle \Psi_H | T\{\hat{\psi}_H(xt)\hat{\psi}^\dagger_H(x't')\}|\Psi_H\rangle}{\langle \Psi_H|\Psi_H\rangle} = \frac{\langle \phi_0 | U(\infty,0)\, T\{\hat{\psi}_H(xt)\hat{\psi}^\dagger_H(x't')\} U(0,-\infty)|\phi_0\rangle}{\langle \phi_0|U(\infty,0)U(0,-\infty)|\phi_0\rangle}$$

also $\quad \hat{O}_H(t) = U(0,t)\,\hat{O}_I(t)\,U(t,0)$

$$\Rightarrow \quad = \frac{\langle \phi_0 | U(\infty,0)\, T\{U(0,t)\hat{\psi}_I(xt)U(t,0)U(0,t')\hat{\psi}^\dagger_I(x't')U(t',0)\}U(0,-\infty)|\phi_0\rangle}{\langle \phi_0|U(\infty,0)U(0,-\infty)|\phi_0\rangle}$$

$$= \frac{\langle \phi_0 | T\{U(\infty,t)\hat{\psi}_I(xt)\,U(t,t')\,\hat{\psi}^\dagger_I(x't')\,U(t',-\infty)\}|\phi_0\rangle}{\langle \phi_0|U(\infty,-\infty)|\phi_0\rangle}$$

$$= \frac{\langle \phi_0 | T\{U(\infty,-\infty)\,\hat{\psi}_I(xt)\,\hat{\psi}^\dagger_I(x',t')\}|\phi_0\rangle}{\langle \phi_0|U(\infty,-\infty)|\phi_0\rangle}$$

Time ordering operator will place all operators at the appropriate places

$$U(\infty,-\infty) = T\left\{e^{i/\hbar\int_{-\infty}^{\infty} dt\, V_I(t)}\right\}$$

Example if $\underline{V=0}$: $\quad G \to G_0$ ← free green's function

$$\frac{\langle \phi_0 | T\{U(\infty,-\infty)\hat{\psi}_I(xt)\hat{\psi}^\dagger_I(x't')\}|\phi_0\rangle}{\langle \phi_0|U(\infty,-\infty)|\phi_0\rangle} \longrightarrow \frac{\langle \phi_0 | T\{\hat{\psi}_I(xt)\hat{\psi}^\dagger_I(x't')\}|\phi_0\rangle}{\langle \phi_0|\phi_0\rangle}$$

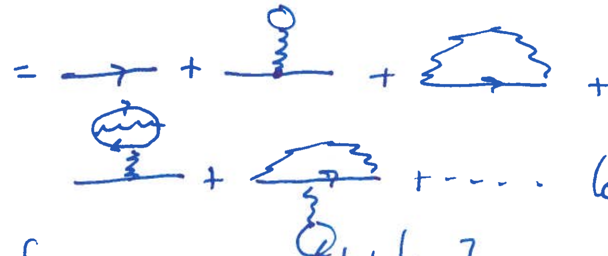
How do we calculate G?

* Diagramatics [Perturbation theory]

$$U(\infty,-\infty) = T\left\{ e^{-i/\hbar \int_{-\infty}^{\infty} d\bar{t}\, V_I(\bar{t})} \right\}$$

$$= \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n\, T\left\{ V_I(t_1) \cdots V_I(t_n) \right\}$$

$$iG(xt, x't') = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n \frac{\langle \phi_0 | T\{ V_I(t_1) \cdots V_I(t_n)\, \hat{\psi}(xt)\, \hat{\psi}^{+}(x't') \} | \phi_0 \rangle}{\langle \phi_0 | U(\infty,-\infty) | \phi_0 \rangle}$$



lots of diagrams need to truncate or perform partial sums!

* Equation of Motion

* Functional Methods [in principle non-perturbative]

– Coherent Path Integrals

→ – Schwinger derivative technique

we will focus on this approach to gain an overview of the subject.

Schwinger Derivative technique & Hedin's equations

~~we start~~

to ~~derive~~ a close form solution we start with

$$iG(1,2) = \langle \Psi_H | T\{ \hat{\psi}_H(1)\, \hat{\psi}^{+}_H(2) \} | \Psi_H \rangle \quad \text{assume } \langle \Psi_H | \Psi_H \rangle = 1$$

composite $x_1 t_1 \equiv 1$

we will now use $\bar{H} = H + \Pi$

full interacting Hamiltonian — a perturbing field

we make no assumption of the adiabatic continuity

Equation of Motion of G

As we have seen, the many-body Hamiltonian in 2nd quantization takes the form

$$\hat{H} = \int d\bar{r}\, \hat{\psi}^{+}(r)\, \underbrace{h(r)}_{-\frac{\hbar^2\nabla^2}{2m} + V_{ne}(r)}\, \hat{\psi}(r) + \frac{1}{2}\int dr \int dr'\, \hat{\psi}^{+}(r)\hat{\psi}^{+}(r')\, \underbrace{v(r,r')}_{\text{Coulomb potential} = \frac{e^2}{|r-r'|}}\, \hat{\psi}(r')\hat{\psi}(r)$$

$-\frac{\hbar^2\nabla^2}{2m}$: kinetic energy; $V_{ne}(r)$: nuclei-electron potential

To start we consider the equation of motion of the annihilation field operator in the Heisenberg picture

$$-i\frac{\partial \hat{\psi}_H(1)}{\partial t_1} = \left[\hat{H}_H(1), \hat{\psi}_H(1)\right] = e^{iHt_1}\left[H, \hat{\psi}(r_1)\right]e^{-iHt_1}$$

Kinetic

$$\left[\hat{H}_{kin}, \hat{\psi}(r_1)\right] = \int dr \left[\hat{\psi}^{+}(r)h(r)\hat{\psi}(r), \hat{\psi}(r_1)\right] = \hat{\psi}^{+}(r)\cancelto{0}{\{h(r)\hat{\psi}(r), \hat{\psi}(r_1)\}} - \{\hat{\psi}^{+}(r)h(r), \hat{\psi}(r_1)\}\hat{\psi}(r)$$

$$= \cancel{\int dr \left(-\delta(r-r_1)\overset{h(r)}{\vee}\hat{\psi}(r)\right)} = \cancel{\int dr\, \delta(r-r_1)\hat{\psi}(r)}$$

$$= -\int dr\, \delta(r-r_1)h(r)\hat{\psi}(r) = -h(r_1)\hat{\psi}(r_1)$$

Interaction

$$\left[\hat{\psi}^{+}(r)\hat{\psi}^{+}(r')\hat{\psi}(r')\hat{\psi}(r), \hat{\psi}(r_1)\right] = \hat{\psi}^{+}(r)\hat{\psi}^{+}(r')\cancelto{0}{\left[\hat{\psi}(r')\hat{\psi}(r), \hat{\psi}(r_1)\right]}$$

$$+ \left[\hat{\psi}^{+}(r)\hat{\psi}^{+}(r'), \hat{\psi}(r_1)\right]\hat{\psi}(r')\hat{\psi}(r)$$

$$= \left(\hat{\psi}^{+}(r)\{\hat{\psi}^{+}(r'), \hat{\psi}(r_1)\} - \{\hat{\psi}^{+}(r), \hat{\psi}(r_1)\}\hat{\psi}^{+}(r')\right)\hat{\psi}(r')\hat{\psi}(r)$$

$$= \hat\psi^\dagger(r)\hat\psi(r')\hat\psi(r)\,\delta(r'-r_1) - \hat\psi^\dagger(r')\hat\psi(r')\hat\psi(r)\,\delta(r-r_1)$$

$$\frac{1}{2}\int dr\int dr'\, v(r,r')\left[\hat\psi^\dagger(r)\hat\psi^\dagger(r')\hat\psi(r')\hat\psi(r),\, \hat\psi(r_1)\right]$$

$$= \frac{1}{2}\left(\int dr\, v(r,r_1)\,\hat\psi^\dagger(r)\hat\psi(r_1)\hat\psi(r) - \int dr'\, v(r_1,r')\,\hat\psi^\dagger(r')\hat\psi(r')\hat\psi(r_1)\right)$$

$r' \to r$

$$= \frac{1}{2}\left(\int dr\, v(r,r_1)\,\hat\psi^\dagger(r)\hat\psi(r_1)\hat\psi(r) - \int dr\, v(r_1,r)\,\hat\psi^\dagger(r)\hat\psi(r)\hat\psi(r_1)\right)$$

swap

$$= \frac{1}{\cancel{2}}\left(\cancel{2}\int dr\, v(r,r_1)\,\hat\psi^\dagger(r)\hat\psi(r_1)\hat\psi(r)\right) \qquad v(r,r') = v(r',r)$$

hermitical & indistinguishability

$$= \int dr\, v(r,r_1)\,\hat\psi^\dagger(r)\hat\psi(r_1)\hat\psi(r)$$

$$-i\frac{\partial \psi_H(1)}{\partial t_1} = e^{iHt_1}\left(-h(r_1)\hat\psi(r_1) + \int dr\, v(r,r_1)\,\hat\psi^\dagger(r)\hat\psi(r_1)\hat\psi(r)\right) \times e^{-iHt_1}$$

$$= -e^{iHt_1}h(r_1)e^{-iHt_1}e^{iHt_1}\hat\psi(r_1)e^{-iHt_1}$$

$$+\int dr\, v(r,r_1)\, e^{iHt_1}\hat\psi^\dagger(r)e^{-iHt_1}e^{iHt_1}\hat\psi(r_1)e^{-iHt_1}e^{iHt_1}\hat\psi(r)e^{-iHt}$$

$$= -h(1)\hat\psi(1) + \int dr\, v(r,r_1)\,\hat\psi^\dagger(r,t_1)\hat\psi(r_1,t_1)\hat\psi(r\,t_1)$$

$$= -h(1)\hat\psi(1) + \int dr\int dt_3\, v(r,r_1)\,\delta(t_3-t_1)\times$$

$$\times\, \hat\psi^\dagger(r\,t_3)\hat\psi(r_1\,t_1)\hat\psi(r\,t_3)$$

$$= -h(1)\hat\psi(1) + \int d3\, v(3,1)\,\hat\psi^\dagger(3)\hat\psi(1)\hat\psi(3)$$

Now we multiply the left hand side by $\langle \Psi_H | T\{$ and the right hand side by $\hat{\psi}^{+}(2)\}|\Psi_H\rangle$

$$-i\,\langle \Psi_H | T\{\frac{\partial}{\partial t_1}\hat{\psi}(1))\,\hat{\psi}^{+}(2)\}|\Psi_H\rangle = -\langle \Psi_H | T\{h(1)\,\hat{\psi}(1)\hat{\psi}^{+}(2)\}|\Psi_H\rangle$$

$$+\int d3\,\langle \Psi_H | T\{v(3,1)\,\hat{\psi}^{+}(3)\hat{\psi}(1)\hat{\psi}(3)\hat{\psi}^{+}(2)\}|\Psi_H\rangle$$

$$\Rightarrow -i\,\langle \Psi_H | T\{\frac{\partial}{\partial t_1}\hat{\psi}(1)\hat{\psi}^{+}(2)|\Psi_H\rangle = -h(1)\,\langle \Psi_H | T\{\hat{\psi}(1)\hat{\psi}^{+}(2)\}|\Psi_H\rangle$$

$$+\int d3\,v(3,1)\,\langle \Psi_H | T\{\hat{\psi}^{+}(3)\hat{\psi}(1)\hat{\psi}(3)\hat{\psi}^{+}(2)\}|\Psi_H\rangle$$

by definition $i\,G(1,2) = \langle \Psi_H | T\{\hat{\psi}(1)\hat{\psi}^{+}(2)\}|\Psi_H\rangle$

$$i^2 G^{(2)}(1,3,3^+,2) = \langle \Psi_H | T\{\hat{\psi}(1)\hat{\psi}(3)\hat{\psi}^{+}(3^+)\hat{\psi}^{+}(2)\}|\Psi_H\rangle$$

when $3^+ = t_3 + 0^+$ ie to recover the ordering $\hat{\psi}^{+}(3)\hat{\psi}(3)$ when time ordering is applied.

to recover G from the left hand side we have

$$i\frac{\partial}{\partial t_1}G(1,2) = \frac{\partial}{\partial t_1}\Big(\theta(1,2)\,\langle \Psi_H|\hat{\psi}(1)\hat{\psi}^{+}(2)|\Psi_H\rangle$$

$$-\theta(2,1)\,\langle \Psi_H|\hat{\psi}^{+}(2)\hat{\psi}(1)|\Psi_H\rangle\Big)$$

$$= \frac{\partial\theta(1,2)}{\partial t_1}\langle \Psi_H|\hat{\psi}(1)\hat{\psi}^{+}(2)|\Psi_H\rangle + \theta(1,2)\,\langle \Psi_H|\frac{\partial}{\partial t_1}\hat{\psi}(1)\,\hat{\psi}^{+}(2)|\Psi_H\rangle$$

$$-\frac{\partial\theta(2,1)}{\partial t_1}\langle \Psi_H|\hat{\psi}^{+}(2)\hat{\psi}(1)|\Psi_H\rangle - \theta(2,1)\,\langle \Psi_H|\hat{\psi}^{+}(2)\frac{\partial\hat{\psi}(1)}{\partial t_1}|\Psi_H\rangle$$

note $\dfrac{\partial\theta(1,2)}{\partial t_1} = -\dfrac{\partial\theta(2,1)}{\partial t_1} = \delta(t_1 - t_2)$

$$\Rightarrow i\frac{\partial}{\partial t_1}G(1,2) = \delta(t_1-t_2)\Big(\langle \Psi_H|\overbrace{\hat{\psi}(1)\hat{\psi}^{+}(2) + \hat{\psi}^{+}(2)\hat{\psi}(1)}^{\delta(r_1 - r_2)}|\Psi_H\rangle\Big)$$

$$+\theta(1,2)\,\langle \Psi_H|\frac{\partial}{\partial t_1}\hat{\psi}(1)\hat{\psi}^{+}(2)|\Psi_H\rangle - \theta(2,1)\,\langle \Psi_H|\hat{\psi}^{+}(2)\frac{\partial}{\partial t_1}\hat{\psi}(1)|\Psi_H\rangle$$

$$\Rightarrow \quad i\frac{\partial}{\partial t_1} G(1,2) = \delta(t_1-t_2)\delta(r_1-r_2) + \langle \Psi_H | T\{ \frac{\partial}{\partial t_1}\psi(1)\, \psi^\dagger(2)\} | \Psi_H \rangle$$

this means

$$-i\left(i\frac{\partial}{\partial t_1} G(1,2) - \delta(1,2) \right) = -h(1)\, i\, G(1,2) + \int d3\, v(3,1)\, (i)^2 G^{(2)}(1,3,3^+,2)$$

$$i\left(\frac{\partial}{\partial t_1} G(1,2) + i\,\delta(1,2) = -ih(1)\, G(1,2) - \int d3\, v(3,1)\, G^{(2)}(1,3,3^+,2) \right)$$

$$i\frac{\partial}{\partial t_1} G(1,2) - \delta(1,2) = h(1)\, G(1,2) - i\int d3\, v(3,1)\, G^{(2)}(1,3,3^+,2)$$

$$\left(i\frac{\partial}{\partial t_1} - h(t) \right) G(1,2) = \delta(1,2) - i\int d3\, v(3,1)\, G^{(2)}(1,3,3^+,2)$$

Here G is defined in terms of $G^{(2)}$ and if we derived the EOM for $G^{(2)}$ it will depend on $G^{(3)}$, and so on. This is the so called Martin–Schwinger hierarchy. To move forward we could truncate this hierarchy which is not controlled, we could resort to Wick's thm, and break each $G^{(n)}$ into its non-interacting parts and do diagrammatics. Here, we will take an alternate path originally used by Schwinger in QED and adapted by Hedin in condensed matter. Namely,

we convert $iG(1,2) = \langle \Psi_H | T\{ \psi_H(1)\, \psi_H^\dagger(2)\} | \Psi_H \rangle$ to the interaction picture. But we do not partition the Hamiltonian into non-interacting & interacting, instead we insert a perturbing field.

$$H \longrightarrow \bar{H} = \underset{\substack{\uparrow \\ \text{full interacting Hamiltonian}}}{H} + \underset{\substack{\uparrow \\ \text{perturbing field.}}}{\Pi}$$

Π is arbitrary and will be set to zero at the end of the analysis so that $U(\infty,-\infty) \to 1$, $\psi_I \to \psi_H$ and $|\Psi_I\rangle \to |\Psi_H\rangle$

so

$$iG(1,2) = \frac{\langle \Psi_I | T\{ U(\infty,-\infty)\, \hat{\psi}_I(1)\, \hat{\psi}_I^{\dagger}(2) \} | \Psi_I \rangle}{\langle \Psi_I | U(\infty,\infty) | \Psi_I \rangle}$$

with

$$U(\infty,-\infty) = T\left\{ e^{-i/\hbar \int_{-\infty}^{\infty} d4\, \hat{\psi}^{\dagger}(4)\, \Pi(4)\, \hat{\psi}(4)} \right\}$$

We will now take the functional derivative of G with respect to Π. To do this we first need $\frac{\delta U}{\delta \Pi}$ since the operators do not depend on Π.

$$\frac{\delta U}{\delta \Pi(3)} = \frac{\delta\, T\left\{ e^{-i/\hbar \int_{-\infty}^{\infty} d4\, \hat{\psi}_I^{\dagger}(4)\, \Pi(4)\, \hat{\psi}_I(4)} \right\}}{\delta \Pi(3)}$$

$$= -i\, T\{ U\, \hat{\psi}_I^{\dagger}(3)\, \hat{\psi}_I(3) \}$$

So,

$$i \frac{\delta G(1,2)}{\delta \Pi(3)} = \frac{\delta}{\delta \Pi(3)} \frac{\langle \Psi_I | T\{ U(\infty,-\infty)\, \hat{\psi}_I(1)\, \hat{\psi}_I^{\dagger}(2) \} | \Psi_I \rangle}{\langle \Psi_I | U(\infty,-\infty) | \Psi_I \rangle}$$

$$\cancel{= -i \frac{\langle \Psi_I | T\{ U(\infty,-\infty)\, \hat{\psi}_I^{\dagger}(3)\, \hat{\psi}_I(3)\, \hat{\psi}_I(1)\, \hat{\psi}_I^{\dagger}(2) | \Psi_I \rangle}{\langle \Psi_I | U(\infty,-\infty) | \Psi_I \rangle}}$$

$$= \frac{\langle \Psi_I | T\{ \frac{\delta U(\infty,-\infty)}{\delta \Pi(3)}\, \hat{\psi}_I(1)\, \hat{\psi}_I^{\dagger}(2) \} | \Psi_I \rangle}{\langle \Psi_I | U(\infty,-\infty) | \Psi_I \rangle} - \frac{\langle \Psi_I | T\{ U(\infty,-\infty)\, \hat{\psi}_I(1)\, \hat{\psi}_I^{\dagger}(2) \} | \Psi_I \rangle}{\langle \Psi_I | U(\infty,-\infty) | \Psi_I \rangle} \times$$

$$\times \frac{\langle \Psi_I | \frac{\delta U(\infty,-\infty)}{\delta \Pi(3)} | \Psi_I \rangle}{\langle \Psi_I | U(\infty,-\infty) | \Psi_I \rangle}$$

$$= -i \frac{\langle \Psi_I | T\{U(\infty,-\infty)\, \hat{\psi}_I^{+}(3)\hat{\psi}_I(3)\hat{\psi}_I(1)\hat{\psi}_I^{+}(2)\}|\Psi_I\rangle}{\langle \Psi_I | U(\infty,-\infty)|\Psi_I\rangle} - (-i)\frac{\langle \Psi_I | T\{U(\infty,-\infty)\hat{\psi}_I(1)\hat{\psi}_I^{+}(2)\}|\Psi_I\rangle}{\langle \Psi_I|U(\infty,-\infty)|\Psi_I\rangle}$$

$$\times \frac{\langle \Psi_I | T\{U(\infty,-\infty)\hat{\psi}_I^{+}(3)\hat{\psi}_I(3)\}|\Psi_I\rangle}{\langle \Psi_I|U(\infty,-\infty)|\Psi_I\rangle}$$

3 permutations

$$= -i(-1)\, i^2 G^{(2)}(1,3,3^+,2) - (-i)\, i\, G(1,2)\,(-1)\, i\, G(3,3^+)$$

1 permutation

$$= -i\, G^{(2)}(1,3,3^+,2) + i\, G(1,2)\, G(3\,3^+)$$

$$= i \frac{\delta G(1,2)}{\delta \pi(3)} \implies \frac{\delta G(1,2)}{\delta\pi(3)} = -G^{(2)}(1,3,3^+,2) + G(1,2)G(3\,3^+)$$

Now we have re-written the 2-particle Green's function in terms of the single particle Green's function and its derivatives. This means,

$$\Big(i\frac{\partial}{\partial t_1} - \underset{-\pi(1)}{h(1)}\Big) G(1,2) = \delta(1,2) - i\int d3\, v(3,1)\left(G(1,2)G(3,3^+) - \frac{\delta G(1,2)}{\delta \pi(3)}\right)$$

$$= \delta(1,2) - i\int d3\; G(3,3^+)\, v(3,1)\, G(1,2)$$

$$+ i\int d3\; v(3,1)\, \frac{\delta G(1,2)}{\delta\pi(3)}$$

Since $G(1\,4)\,G^{-1}(4,2) = \delta(1,2)$

$$\frac{\delta}{\delta\pi(3)}\big(G(1,4)\,G^{-1}(4,2)\big) = 0 \implies \frac{\delta G(1,2)}{\delta\pi(3)} = -G(1,4)\frac{\delta G^{-1}(4,5)}{\delta\pi(3)}G$$

So,

$$\Big(i\frac{\partial}{\partial t_1} - \underset{-\pi(1)}{h(1)}\Big) G(1,2) = \delta(1,2) - i\int d3\, G(3,3^+)\, v(3,1)\, G(1,2)$$

$$- i\int d3\; v(3,1)\, G(1,4)\frac{\delta G^{-1}(4,5)}{\delta \pi(3)} G(5,2)$$

we recognize that $iG(3,3^+) = -\rho(3)$ (the density)

and $\int d3\, \rho(3)\, v(3,1) = V_H(1)$ the Hartree potential.

$$\Big(\underbrace{i\frac{\partial}{\partial t_1} - h(1)\overset{-\pi(1)}{\downarrow}}_{G_0^{-1}}\Big) G(1,2) = \delta(1,2) + V_H(1)\, G(1,2) - i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta G^{-1}(4,5)}{\delta \pi(3)}\, G(5,2)$$

$$= \delta(1,2) + \Big(\underbrace{V_H(1)\,\delta(1,5) - i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta G^{-1}(4,5)}{\delta \pi(3)}}_{\Sigma \,\equiv\, \Sigma_{Hartree} + \Sigma_{xc}}\Big) G(5,2)$$

self energy

$$G_0^{-1}(1,3)\, G(3,2) = \delta(1,2) + \Sigma(1,5)\, G(5,2)$$

$$G(1,2) = G_0(1,2) + G_0(1,4)\, \Sigma(4,5)\, G(5,2) \quad \text{Dyson's Eq.}$$

or

$$G^{-1}(1,2) = G_0^{-1}(1,2) - \Sigma(1,2)$$

Typically the Hartree contribution is added to the bare green's func.

$$\Big(\underbrace{i\frac{\partial}{\partial t_1} - h(1) - V_H(1)\overset{-\pi(1)}{\downarrow}}_{G_H^{-1}}\Big) G(1,2) = \delta(1,2) + \Sigma(1,5)\, G(5,2)$$

we now focus on the self-energy,

$$\Sigma(1,5) = -i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta G^{-1}(4,5)}{\delta \pi(3)}$$

if we substitute G^{-1} into Σ

$$\Sigma(1,5) = -i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta}{\delta \pi(3)}\Big[G_0^{-1}(4,5) - \Sigma(4,5)\Big]$$

$$= -i\int d3\, v(3,1)\, G(1,4)\left(\frac{\delta G_0^{-1}(4,5)}{\delta \pi(3)} - \frac{\delta \Sigma(4,5)}{\delta \pi(3)}\right)$$

$$\frac{\delta G_0^{-1}(4,5)}{\delta\Pi(3)} = \frac{\delta}{\delta\Pi(3)}\left(i\frac{\partial}{\partial t_1} - h(4) - V_H(4) - \Pi(4)\right)\delta(4,5)$$

$$= \left(-\frac{\delta V_H(4)}{\delta\Pi(3)} - \delta(4,3)\right)\delta(4,5)$$

$$\Sigma(1,5) = -i\int d3\, v(3,1)\, G(1,4)\left(-\frac{\delta V_H(4)}{\delta\Pi(3)}\delta(4,5) - \delta(4,3)\delta(4,5) - \frac{\delta\Sigma(4,5)}{\delta\Pi(3)}\right)$$

$$= +i\int d3\, \delta(4,3)\,\delta(4,5)\, v(3,1)\, G(1,4)$$

$$+ i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta V_H(4)}{\delta\Pi(3)}\,\delta(4,5)$$

$$+ i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta\Sigma(4,5)}{\delta\Pi(3)}$$

$$= +i\, v(5,1)\, G(1,5) + i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta V_H(5)}{\delta\Pi(3)}$$

$$+ i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta\Sigma(4,5)}{\delta\Pi(3)}$$

Exchange ~~sigh~~ but with G inside of G_0

This is an iteration equation for the self-energy which provides a procedure for making an expansion of the self-energy in powers of the Coulomb interaction.

Exercise find Σ to second order in v.

$$\frac{\delta V_H(5)}{\delta\Pi(3)} = \int d9\, \frac{\delta\rho(9)}{\delta\Pi(3)}\, v(9,5) = -i\int d9\, \frac{\delta G(99^+)}{\delta\Pi(3)}\, v(9,5)$$

$$= +i\int d9\, G(9,10)\, \frac{\delta G^{-1}(10,11)}{\delta\Pi(3)}\, G(11,9^+)\, v(9,5)$$

to first order in v, $\frac{\delta G^{-1}(10,11)}{\delta\Pi(3)} = -\delta(10,3)\,\delta(10,11)$

$$\frac{\delta V_H(5)}{\delta\Pi(3)} \simeq -i\int d9\, G(9,3)\, G(3,9^+)\, v(9,5)$$

thus $\frac{\delta\Sigma(4,5)}{\delta\bar{v}(3)}$ to first order in v, is

$$\frac{\delta\Sigma(4,5)}{\delta\bar{v}(3)} = +i\,v(5,4)\,\frac{\delta G(4,5)}{\delta\bar{v}(3)}$$

$$= -i\,v(5,4)\,G(4,13)\underbrace{\frac{\delta G^{-1}(13,14)}{\delta\bar{v}(3)}}_{-\delta(13,3)\,\delta(13,14)}G(14,5)$$

$$= +i\,v(5,4)\,G(4,3)\,G(3,5)$$

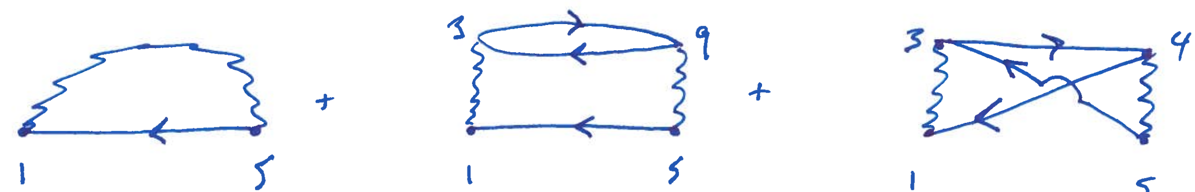
thus

$$\Sigma(1,5) = +i\,v(5,1)\,G(1,5) + i\int d3\, v(3,1)\,G(1,5)\left[-i\int d9\, G(9,3)\,G(3,9^{+})\,v(9,5)\right]$$

$$+\, i\int d3\, v(3,1)\,G(1,4)\left(+i\,v(5,4)\,G(4,3)\,G(3,5)\right)$$

$$= i\,v(5,1)\,G(1,5) + \int d3\int d9\,(i)\,v(3,1)\,G(1,5)\,G(9,3)\,G(3,9^{+})\,(-i)\,v(9,5)$$

$$+ \int d3\, i\,v(3,1)\,G(1,4)\,i\,v(5,4)\,G(4,3)\,G(3,5)$$

$\Sigma =$ 

1st order exchange + 2-rung ladder + 2nd order exchange

the Schwinger derivative technique has several advantages over the conventional diagrammatic technique. The integration equation for the self energy is exact and it allows us to generate all the terms in the perturbation expansion without the need to enumerate topologically distinct connected diagrams and to employ the tedious ~~which~~ Wick's theorem. Moreover, the ground state in the definition of the Green's function in the interaction picture is the exact interacting groundstate thus is no assumption of adiabatic continuity associated with switching on the Coulomb interaction from $t=\pm\infty$ to $t=0$, that is needed to make a one-to-one connection between the non-interacting groundstate and the interacting one. The probing field in the functional derivative technique can be large and rapidly varying in time. its role is to perturb the response of the system, next to its current a non-vibrating and interacting ground state, the Schwinger functional derivative technique provides a simple & elegant way of deriving the self energy.

the self-energy ~~xx~~ at the end of this section (expansion in v) leads to unphysical results in solids. the reason is that screening effects in solids are of great importance. at low energies the effective Coulomb interaction is much smaller than the bare value, especially in metals. It was than proposed by Lars Hedin to expand the self energy in powers of the screened interaction rather than the bare Coulomb interaction, since W is much weaker it is expected to converge faster. though this is not the case the resulting set of equations proved a powerful basis for examining electronic structure of matter from first-principles.

The key: instead of taking derivatives in Σ w.r.t. π we work in the total field:

$$\Phi = \pi + V_H$$

this means

$$\Sigma(1,5) = i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta G^{-1}(4,5)}{\delta\pi(3)}$$

$$= i\int d3\, v(3,1)\, G(1,4)\, \frac{\delta G^{-1}(4,5)}{\delta\Phi(6)} \cdot \frac{\delta\Phi(6)}{\delta\pi(3)}$$

ratio of total and applied field $\equiv \varepsilon^{-1}$ (longitudinal)

$$\Sigma(1,5) = i\int d3\, \frac{\delta\Phi(6)}{\delta\pi(3)} v(3,1)\, G(14)\, \frac{\delta G^{-1}(4,5)}{\delta\Phi(6)}$$

let $$\int d3\, \frac{\delta\Phi(6)}{\delta\pi(3)} v(3,1) = \int d3\, \varepsilon^{-1}(6,3)\, v(3,1) = W(6,1)$$

also

$$W(6,1) = \frac{\delta\Phi(6)}{\delta\pi(3)} v(3,1) = \left(\frac{\delta\pi(6)}{\delta\pi(3)} + \frac{\delta V_H(6)}{\delta\pi(3)}\right) v(3,1)$$

$$= \left(\delta(6,3) + \frac{\delta\rho(4)}{\delta\pi(3)} v(4,6)\right) v(3,1)$$

$$= \left(\delta(6,3) + \frac{\delta\varphi(4)}{\delta\Phi(7)} \cdot \frac{\delta\Phi(7)}{\delta\pi(3)} v(4,6)\right) v(3,1)$$

$$= \left(\delta(6,3) + v(6,4)\, P(4,7)\, \frac{\delta\Phi(7)}{\delta\pi(3)}\right) v(3,1)$$

$$= v(6,1) + v(6,4)\, P(4,7)\, W(7,1)$$

$$P(4,7) = \frac{\delta\rho(4)}{\delta\Phi(7)} = -i\,\frac{\delta G(44^+)}{\delta\Phi(7)} = +i\, G(4,8)\, \frac{\delta G^{-1}(8,9)}{\delta\Phi(7)}\, G(9,4^+)$$

$$= -i\, G(4,8)\, \Gamma(8,9;7)\, G(9,4^+)$$

$$\Gamma(4,5;6) = -\frac{\delta G^{-1}(4,5)}{\delta\Phi(6)} = -\frac{\delta\left(i\frac{\partial}{\partial t_4}\delta(4,5) - h(4)\delta(4,5) - \Phi(4)\delta(4,5) - \Sigma(4,5)\right)}{\delta\Phi(6)}$$

$$= -\left(-\delta(4,6)\,\delta(4,5) - \frac{\delta\Sigma(4,5)}{\delta\Phi(6)}\right)$$

$$= \delta(4,6)\,\delta(4,5) + \frac{\delta\Sigma(4,5)}{\delta G(7,8)}\,\frac{\delta G(7,8)}{\delta\Phi(6)}$$

$$= \delta(4,6)\,\delta(4,5) - \frac{\delta\Sigma(4,5)}{\delta G(7,8)}\, G(7,9)\, \frac{\delta G^{-1}(9,10)}{\delta\Phi(6)}\, G(10,8)$$

$$\Gamma(4,5;6) = \delta(4,6)\,\delta(4,5) + \frac{\delta\Sigma(4,5)}{\delta G(7,8)}\, G(7,9)\,\Gamma(9,10;6)\,G(10,8)$$

so all together

$$\Sigma(4,5) = -i\, W(6,1)\, G(1,4)\, \Gamma(4,5;6)$$

W: screened interaction (response of system)

Γ: vertex (all other interactions between quasiparticles)

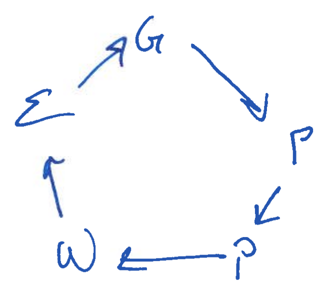
$$\Gamma(4,5;6) = \delta(4,6)\,\delta(4,5) + \frac{\delta\Sigma(4,5)}{\delta G(7,8)}\, G(7,9)\,\Gamma(9,10;6)\,G(10,8)$$

$$W(6,1) = v(6,1) + v(6,4)\, P(4,7)\, W(7,1)$$

$$P(4,7) = -i\, G(4,8)\, \Gamma(8,9;7)\, G(9,4^{+})$$

$$G(1,2) = G_0(1,2) + G_0(1,3)\, \Sigma(3,4)\, G(4,2)$$

* →



Approximations:

Assume $\Gamma = \delta$
- scGW
- G_0W_0
- qpGW

Assume a diagrammatic form for Γ
- $GW\Gamma_1$
- $GW\Gamma_{GW}$
- GWT
- GT (T-matrix)

Assume $\Sigma = \Sigma_{loc}$
- DMFT

assume $\Gamma = \Gamma_{loc}$
- DPA

Assume $\Gamma = \delta$ & $W = v$
- (Fock exchange) vG

* we have achieved a major reduction of the equations needed to determine G: from an infinite set of the Martin-Schwinger hierarchy to five Hedin's equations.

Exercise

Determine the GW correction to the vertex P, and the next iteration for GW approximation $\Sigma(1,5) = -i W(5,1) G(1,5)$ of Σ.

because $P(4,5;6) = \delta(4,6)\,\delta(4,5)$.

Now we need $\dfrac{\delta \Sigma(4,5)}{\delta G(7,8)}$

$$\frac{\delta \Sigma(4,5)}{\delta G(7,8)} = \frac{\delta}{\delta G(7,8)}\Big(-i W(5,4) G(4,5)\Big)$$

$$= -i\left(\frac{\delta W(5,4)}{\delta G(7,8)} G(4,5) + W(5,4)\frac{\delta G(4,5)}{\delta G(7,8)}\right)$$

$$= -i\left(\frac{\delta W(5,4)}{\delta G(7,8)} G(4,5) + W(5,4)\,\delta(4,7)\,\delta(5,8)\right)$$

$$\frac{\delta W(5,4)}{\delta G(7,8)} = \frac{\delta}{\delta G(7,8)}\Big(v(5,4) + v(5,6) P(6,9) W(9,4)\Big)$$

$$= v(5,6)\left(\frac{\delta P(6,9)}{\delta G(7,8)} W(9,4) + P(6,9)\frac{\delta W(9,4)}{\delta G(7,8)}\right)$$

$$= v(5,6)\frac{\delta P(6,9)}{\delta G(7,8)} W(9,4) + v(5,6) P(6,9)\frac{\delta W(9,4)}{\delta G(7,8)}$$

$$\frac{\delta W(5,4)}{\delta G(7,8)} - v(5,6) P(6,9)\frac{\delta W(9,4)}{\delta G(7,8)} = v(5,6)\frac{\delta P(6,9)}{\delta G(7,8)} W(9,4)$$

$$\underbrace{\Big(\delta(5,9) - v(5,6) P(6,9)\Big)}_{\mathcal{E}(5,9)}\frac{\delta W(9,4)}{\delta G(7,8)} = v(5,6)\frac{\delta P(6,9)}{\delta G(7,8)} W(9,4)$$

$$\frac{\delta W(9,4)}{\delta G(7,8)} = \mathcal{E}^{-1}(9,5)\, v(5,6)\frac{\delta P(6,10)}{\delta G(7,8)} W(10,4) = W(9,6)\frac{\delta P(6,10)}{G(7,8)} W(10,4)$$

$$\frac{\delta P(6,10)}{\delta G(7,8)} = -i \frac{\delta}{\delta G(7,8)} \Big(G(6,10)\, G(10,6^+) \Big)$$

$$= -i \Big(\delta(7,6)\, \delta(8,10)\, G(10,6^+) + G(6,10)\, \delta(10,7)\, \delta(6^+,8) \Big)$$

$$\frac{\delta W(9,4)}{\delta G(7,8)} = W(9,6) \Big[-i\, \delta(7,6)\, \delta(8,10)\, G(10,6^+) + G(6,10)\, \delta(10,7)\, \delta(6^+,8) \Big] W(10,$$

$$= -i W(9,6)\, G(10,6^+)\, W(10,4)\, \delta(7,6)\, \delta(8,6)$$

$$- i W(9,6)\, G(6,10)\, W(10,4)\, \delta(10,7)\, \delta(6^+,8)$$

$$= -i\ W(9\ 7)\, G(8\ 7)\, W(8\ 4) - i W(9\ 8)\, G(8\ 7)\, W(7\ 4)$$

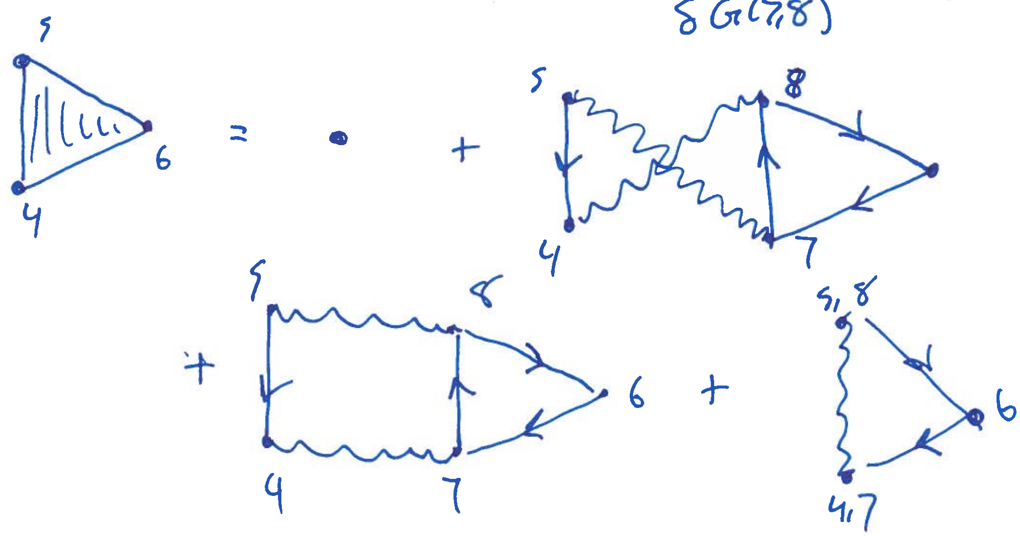
$$\frac{\delta \Sigma(4,5)}{\delta G(7,8)} = -i \Big(-i W(9,7) G(8,7) W(8\ 4) \overset{G(4,5)}{} - i W(9,8) G(8,7) W(7,4) G(4,5)$$

$$+ W(5,4)\, \delta(4,7)\, \delta(5,8) \Big)$$

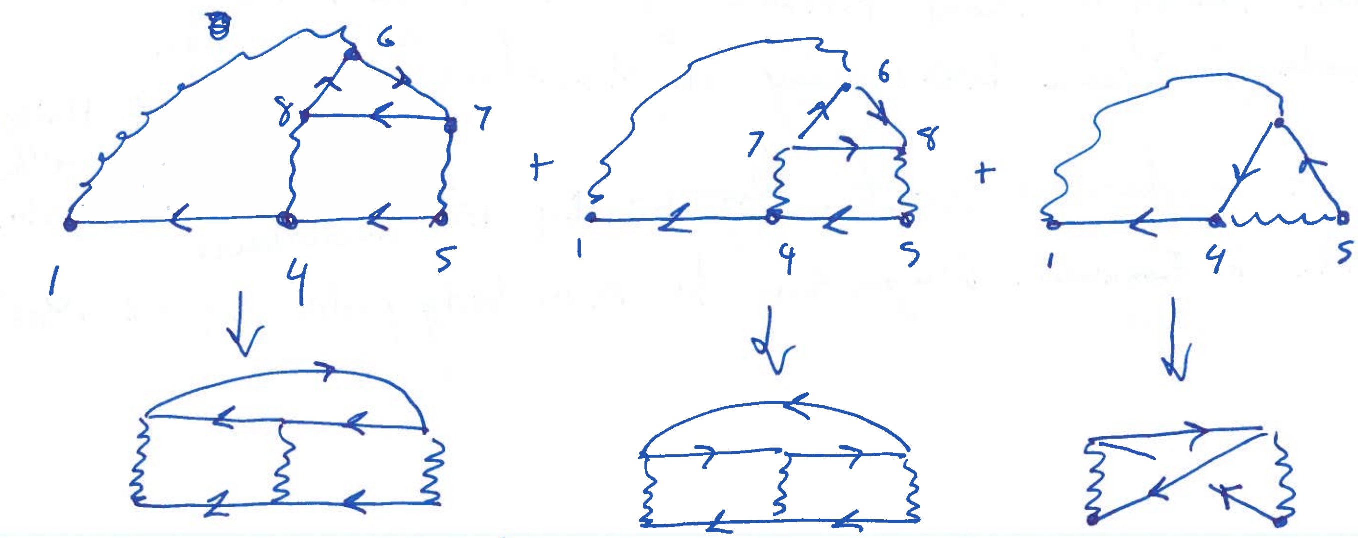
$$= (-i) W(9,7)\, G(8,7)\, (-i) W(8,4) + (-i) W(9,8)\, G(8,7)\, (-i) W(7,4)$$

$$+ (-i) W(5,4)\, \delta(4,7)\, \delta(5,8)$$

$$P(4,5,6) = \delta(4,6)\, \delta(4,5) + \frac{\delta \Sigma(4,5)}{\delta G(7,8)} G(7,6)\, G(6,8)$$



$$\Sigma(1,5) = -i\, W(6,1)\, G(1,4)\, P(4,5;6)$$



3-rung particle-particle ladder

3 rung particle-hole ladder

2nd order exchange.

References

Nonequilibrium Many-body theory of Quantum systems by G. Stefanucci, R. van Leeuwen

Quantum Theory of Many-Particle systems by AL Fetter, JD Walecka

Methods of Quantum Field theory in statistical physics AA. Abrikosov, LP Gor'kov, IE Dzyaloshinski

Green's Functions in Quantum Physics by EN Economou

A Guide to Feynman Diagrams in the Many-body problem by RD Mattuck

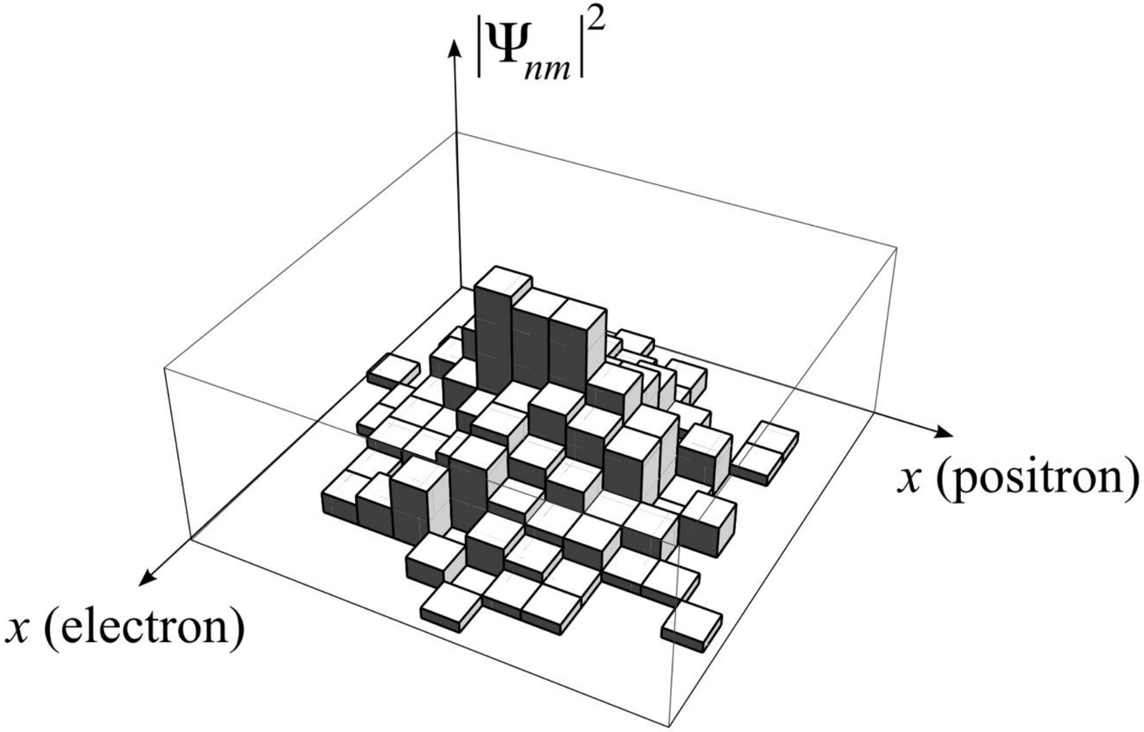


Figure 1.2 Histogram of the normalized number of simultaneous clicks of the electron and positron detectors in $x_n = n\Delta$ and $x_m = m\Delta$ respectively. The height of the function corresponds to the probability $|\Psi_{nm}|^2$.

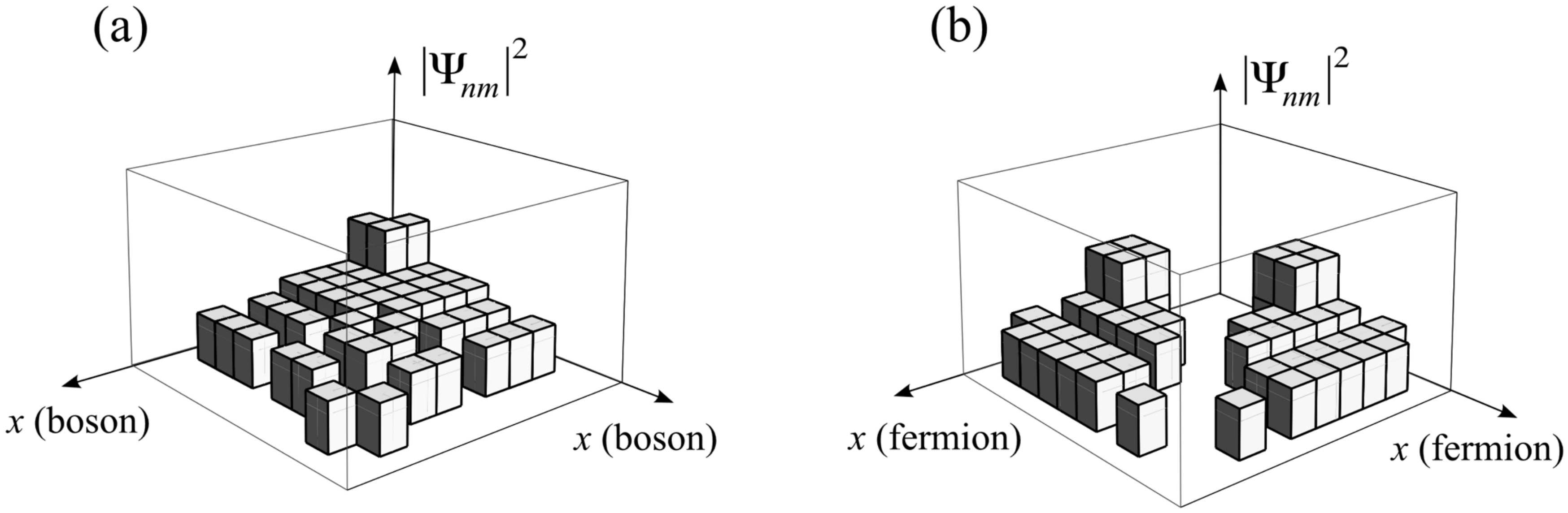


Figure 1.3 Histogram of the normalized number of simultaneous clicks of the detector in $x_n = n\Delta$ and in $x_m = m\Delta$ for (a) two bosons and (b) two fermions. The height of the function corresponds to the probability $|\Psi_{nm}|^2$.

TABLE A.1. Correspondence of single-particle operators in the coordinate and occupation number representations.

Physical observable	Coordinate representation	Occupation number representation	Momentum basis[§]
Particle density at $\boldsymbol{r}$	$\sum_i \delta(\boldsymbol{r}_i - \boldsymbol{r})$	$\psi^+(\boldsymbol{r})\psi(\boldsymbol{r})$	$\sum_{\boldsymbol{k},\boldsymbol{q},\sigma} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}+\boldsymbol{q}\sigma} \exp(i\boldsymbol{q}.\boldsymbol{r})$
Total number of particles	$\sum_i 1 = N$	$\int d^3r\, \psi^+(\boldsymbol{r})\psi(\boldsymbol{r})$	$\sum_{\boldsymbol{k},\sigma} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$
Charge density at $\boldsymbol{r}$	$e\sum_i \delta(\boldsymbol{r}_i - \boldsymbol{r})$	$e\psi^+(\boldsymbol{r})\psi(\boldsymbol{r})$	$e\sum_{\boldsymbol{k},\boldsymbol{q},\sigma} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}+\boldsymbol{q}\sigma} \exp(i\boldsymbol{q}.\boldsymbol{r})$
Current density at $\boldsymbol{r}$	$\frac{e}{2m}\sum_i [\boldsymbol{p}_i\delta(\boldsymbol{r}_i - \boldsymbol{r}) + \delta(\boldsymbol{r}_i - \boldsymbol{r})\boldsymbol{p}_i]$	$\frac{-ie}{2m}[\psi^+(\boldsymbol{r})\nabla\psi(\boldsymbol{r}) - \{\nabla\psi^+(\boldsymbol{r})\}\psi(\boldsymbol{r})]$	$\frac{e}{2m}\sum_{\boldsymbol{k},\boldsymbol{q},\sigma} (2\boldsymbol{k}+\boldsymbol{q}) c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}+\boldsymbol{q}\sigma} \exp(i\boldsymbol{q}.\boldsymbol{r})$
Kinetic energy	$\sum_i p_i^2/2m \equiv -\sum_i \nabla_i^2/2m$	$-\frac{1}{2m}\int d^3r\, \psi^+(\boldsymbol{r})\nabla^2\psi(\boldsymbol{r})$	$\sum_{\boldsymbol{k},\sigma} \frac{k^2}{2m} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$
Potential energy in an external potential $V(\boldsymbol{r})$	$\sum_i V(\boldsymbol{r}_i)$	$\int d^3r\, \psi^+(\boldsymbol{r})V(\boldsymbol{r})\psi(\boldsymbol{r})$	$\mathscr{V}^{-1}\sum_{\boldsymbol{k},\boldsymbol{q},\sigma} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}+\boldsymbol{q},\sigma} \int d^3r\, V(\boldsymbol{r}) \exp(i\boldsymbol{q}.\boldsymbol{r}$
Magnetic moment density at $\boldsymbol{r}$[†]	$(g/2)\ \sum_i \boldsymbol{\sigma}_i \delta(\boldsymbol{r}_i - \boldsymbol{r})$	$(g/2)\psi^+(\boldsymbol{r})\boldsymbol{\sigma}\psi(\boldsymbol{r})$	$(g/2)\sum_{\boldsymbol{k},\boldsymbol{q},\sigma} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}+\boldsymbol{q}\sigma'} \exp(i\boldsymbol{q}.\boldsymbol{r}) u^+_\sigma \boldsymbol{\sigma} u_{\sigma'}$
Total magnetic moment[†]	$(g/2)\sum_i \boldsymbol{\sigma}_i$	$(g/2)\int d^3r\, \psi^+(\boldsymbol{r})\boldsymbol{\sigma}\psi(\boldsymbol{r})$	$(g/2)\sum_{\boldsymbol{k},\sigma,\sigma'} c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma'} u^+_\sigma \boldsymbol{\sigma} u_{\sigma'}$

[†] g is the gyromagnetic ratio of the particles and $\sigma_x, \sigma_y, \sigma_z$ are the 2×2 Pauli matrices.

[§] The expressions are written for particles possessing spin. For particles which do not, the spin label should be ignored.

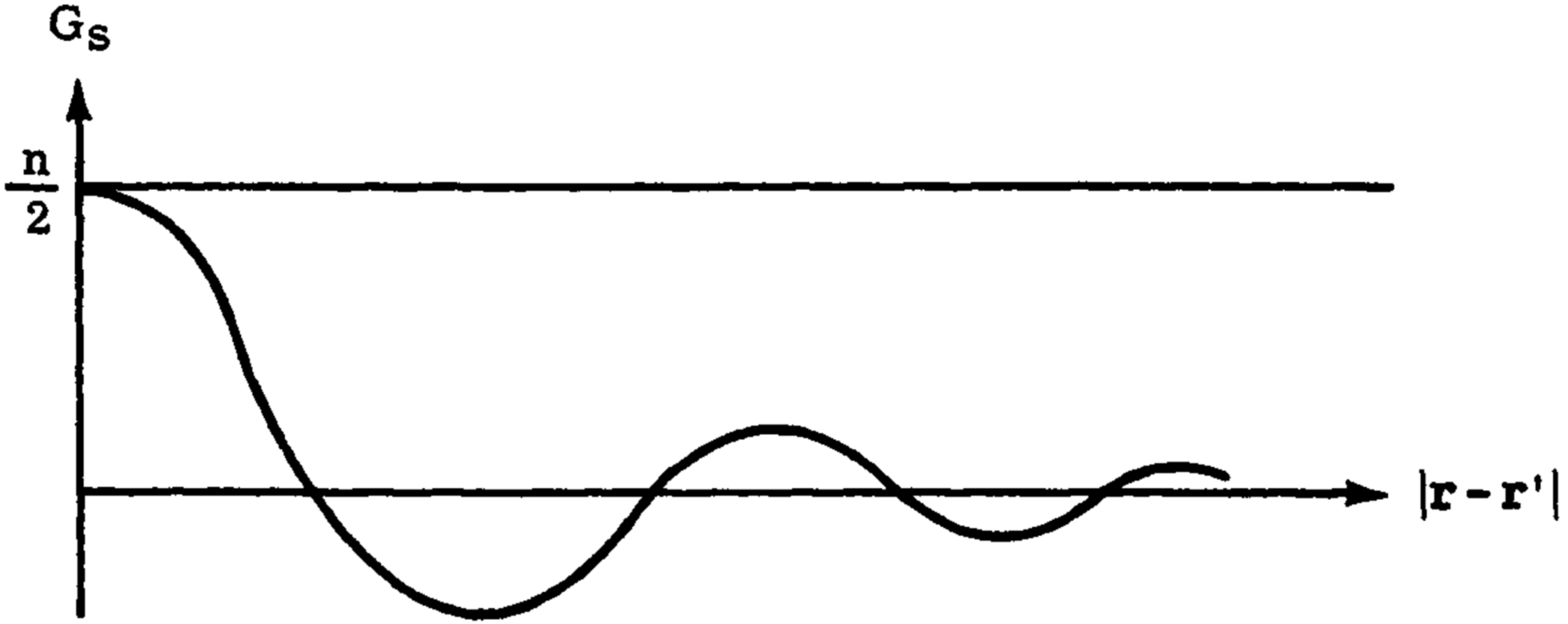
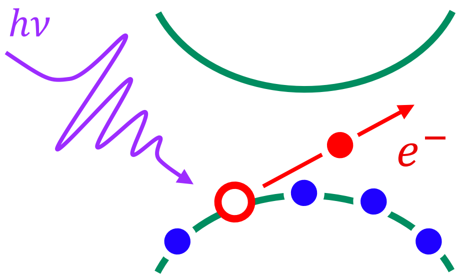
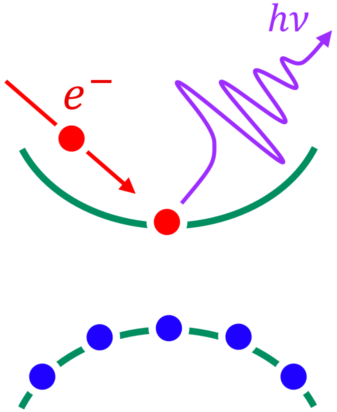


Fig. 19-1

The one-particle density matrix G_s for noninteracting spin ½ fermions.



Direct Photoemission: N ⟶ N-1



Inverse Photoemission: N ⟶ N+1