Ergänzende Bemerkungen zur Vorlesung:

Ausgewählte Kapitel der Theoretischen Physik: Feynman Diagramme

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WS 2007

Version V1.0, January 2007

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1 Introduction

Aim:

- message: one can really compute with theses things
- proper definition
- some general concepts
- some famous approximations
- the work of Sottile
- parquet diagrams

ad 1.) not just (but, of course, also) good for illustration
ad 2.) to come
ad 3.) e.g. linked cluster theorem, fctal derivative wrt ext pot, etc ad 4.) e.g. RPA, Bethe–Salpeter, GW ad 5.) aiming at overlap 2p2h ↔ TDHF ad 6.) (kro)

too simple ↔ to adavced:
will be both . . . (I'll try to adress students as well as PhD people)

Mattuck:
,,A 0th and 1st chapter have been added which are on the pre-kindergarten or nursery school level."
→ homeworks

0.0 Basics

0.0.1 2 examples of calculating with pictures

(Bsp) geometric series $1 + \frac{1}{2} + \frac{1}{4} + \frac{1}{8} + \frac{1}{16} + \ldots$

(Bsp) red wine in white wine

Of course, for *quantitative* conclusions, each pic must be clearly in a 1:1 correspondence with an explicit quantity

sometimes: ,,virtual intermediate states" $\longrightarrow$ perturbation theory ($\equiv$ PT) $\rightarrow$ homeworks

0.0.2 perturbation theory & notation conventions

necessary: (nona) a system + a perturbation:

$$H = \underset{E_{\text{kin}}}{T} + V + U$$

interaction $\equiv$WW: $\sum i < jv(|\mathbf{r}_i - \mathbf{r}_j|) = \sum v(r_{ij})$ e.g. Coulomb, LJ, ...
ext.potential: e.g. substrate, ion lattice, ,,film" (well), **inhom**. system, there can be an intrinsically inhom system (eg electrons in crystal) subject to an additional external perturbation (eg electrostatic potential)

here: convention

$$\boxed{\begin{array}{rcccc} H^{\text{ges}} = & T & +V & +U & +H^{\text{ext}} \\ = & E_{\text{kin}} & \text{WW} & \text{inhom} & \text{ext.pert.} \end{array}} \qquad \begin{array}{c} H^{\text{ext}} = U^{\text{ext}} \\ H^0 = T \end{array} \tag{1}$$

perturbation th:

- with respect to interaction: ,,$H = H^0 + V$" ... $H^0 = T + U$, ,,$V = V$ (WW)"
  $\longrightarrow$ typically for diagrams
- with respect to ext.perturb: ,,$H = H^0 + V$" ... $H^0 = T + V$, ,,$V = U^{\text{ext}}$ (ext. switch))"
  $\longrightarrow$ typically for diagrams lin response

here:

$$H^0 = T \qquad \begin{array}{rcccl} H^{\text{ges}} & = & (T+U) + V & =: & \widetilde{H}^0 + V \\ H^{\text{ges}} & = & (T+U+V) + U^{\text{ext}} & =: & \widetilde{H}^0 + U^{\text{ext}} \end{array} \tag{2}$$

0.0.3 many particles: occupation number formalism

generally well–known: interacting many–body (=many–particle) =MB problem insoluble, non–interacting case = solvable (apart from numerics)
statistic!

(Bsp) 2 spinless 1dim H.O. w.o. interaction: $\widetilde{H}^0 = \widehat{\widetilde{H}}^0 = \hat{h}_1 + \hat{h}_2$

3 HOs: Fermions $\Phi(x_1, x_2, x_3) = \ldots =: \frac{1}{\sqrt{3!}}\|\phi_{\nu_i}(x_j)\| =: \frac{1}{\sqrt{N!}}\|\phi_i(j)\|$
ground state:

3 HOs: Bosons with same energy: wve fct explicitly $\rightarrow$ homework

the info ,,Bosons" & ,,which single–particle levels occupied" = enough! (completely irrelevant, which particle in which level) $\Rightarrow$

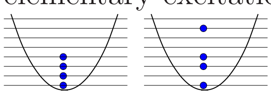
$$\Phi_{\nu_1,\nu_2,\nu_3} \;\rightarrow\; \begin{array}{l} \Phi_{n_1,n_2,n_3,n_4,n_5,\ldots} \\ =: \left|n_1, n_2, n_3, n_4, n_5, \ldots\right\rangle \end{array} \qquad \begin{array}{l} n_i \ldots \ \#\text{ of particles in level } i \\ \sum_i n_i = N \text{ total } \#\text{ of particles} \end{array} \qquad n_i^0 = \frac{1}{e^{\beta(\varepsilon_i - \mu)} \pm 1}$$

temperature $T = 0$: Fermions $n_i = \{0, 1\}$.

ground state:

$$\Phi_0 \;=\; \begin{array}{ll} \text{Bosons:} & \text{all in lowest } \phi_0 \\ \text{Fermions:} & \|N \text{ lowest } \phi_i\| \end{array}$$

elementary excitations of particles and holes:



Φ_{ph}

convention: (kro)

$$\begin{array}{llll} h, h', h'', \ \ldots \ , h_1, h_2, \ \ldots & \text{,,hole" indices, } i.e. & n_h = 1 & \\ p, p', p'', \ \ldots \ , p_1, p_2, \ \ldots & \text{,,particle" indices,} & n_p = 0 & n_p^- := \overline{n}_p := (1 - n_p) = 1 \end{array} \tag{3}$$

creation & annihilation operators:

$a_k^\dagger\, \Phi_0$ ... creates 1 additional particle in level k if there is room
$a_k\, \Phi_0$ ... destroys 1 particle in level k if there is one

Bsp $a_p^\dagger\, \Phi_0$,

$a_h\, \Phi_0$,
$a_p\, \Phi_0$,
$a_h^\dagger\, \Phi_0$

Bsp $a_k^\dagger a_k\, \Phi_0$,

$\widehat{N}$

Bsp $H^0 = T$ (kinetic energy operator) or $\widetilde{H}^0 \rightarrow$ homework

0.1 $n-$particle states

vacuum state:
no particles present $\longrightarrow$ no levels occupied $\Phi \equiv \Phi_{\mathrm{V}}$

single–particle states:
a definite level k_0 occupied: $\Phi = \big|0, \ldots, 1, 0, \ldots\big\rangle \;=\; a^{\dagger}_{k_0}\, \Phi_{\mathrm{V}} \;\equiv\; \Phi_{k_0}$
$\rightarrow$ homework

$$\big[a^{\dagger}_{k_1}, a_{k_2}\big]_{\pm} = \delta_{k_1,k_2}$$

some level k occupied with propability $w_k = |f_k|^2$: $\Phi = \Phi^{(1)}$

two–particle states:
2 definite levels k_1, k_2 occupied: $\Phi = \big|0, \ldots, 1, 0, \ldots, 1, 0, \ldots\big\rangle \;=\; a^{\dagger}_{k_1}\, a^{\dagger}_{k_2}\, \Phi_{\mathrm{V}} \;\equiv\; \Phi_{k_1,k_2}$
must be (antisymm.) wrt interparticle exchange $\Rightarrow$

$$\big[a^{\dagger}_{k_1}, a^{\dagger}_{k_2}\big]_{\pm} = 0 \quad \Rightarrow \quad \big[a_{k_1}, a_{k_2}\big]_{\pm} = 0$$

some levels k_1, k_2 occupied: $\Phi = \Phi^{(2)}$

$N-$particle states:
analogously: $\boxed{\Phi \;=\; \Phi_{k_1\ldots,k_N} \;=\; a^{\dagger}_{k_1} \ldots a^{\dagger}_{k_N}\, \Phi_{\mathrm{V}}}$
or, more generally, $= \Phi^{(N)} = \sum_{k_1\ldots,k_N} f_{k_1\ldots,k_N}\, \Phi_{k_1\ldots,k_N}\,.$

$N-$particle ground state:
Bosons: $\Phi_0 \;=\; \left(a^{\dagger}_{h_0}\right)^N \Phi_{\mathrm{V}}$
Fermions: $\Phi_0 \;=\; a^{\dagger}_{h_0} \ldots a^{\dagger}_{h_{\mathrm{F}}}\, \Phi_{\mathrm{V}}$

expectation values:
trivially $\langle \Phi_{\mathrm{V}} | \Phi_{\mathrm{V}} \rangle = 1$
single–particle states: $\langle \Phi^{(1)} | \Phi_{\mathrm{V}} \rangle = \langle a^{\dagger} \Phi_{\mathrm{V}}\, | \Phi_{\mathrm{V}} \rangle \;=\; \langle \Phi_{\mathrm{V}} |\, a \Phi_{\mathrm{V}} \rangle = 0$
$\langle \Phi_{k_1} | \Phi_{k_2} \rangle \;=\; \langle a^{\dagger}_{k_1}\, \Phi_{\mathrm{V}}\, |\, a^{\dagger}_{k_2} \Phi_{\mathrm{V}} \rangle \;=\; \langle \Phi_{\mathrm{V}}\, |\, a_{k_1} a^{\dagger}_{k_2} \Phi_{\mathrm{V}} \rangle \;=\; \ldots$

two–particle states: $\langle \Phi^{(2)} | \Phi_{\mathrm{V}} \rangle = 0 \quad ; \quad \langle \Phi^{(2)} | \Phi^{(1)} \rangle = 0$
$\langle \Phi_{k_1,k_2} | \Phi_{k'_1,k'_2} \rangle \;=\; \ldots \;\equiv\; \mathcal{A} \delta_{k_1,k'_1} \delta_{k_2,k'_2}$

ground state expectation values:
$\rightarrow$ homeworkMartin

0.2 $n-$particle properties

0.2.1 single–particle properties

any property $A^{(1)}$, that 1 particle can have (e.g. momentum, ...)
measured vaues $A_\alpha = A_0, A_1, \ldots$

elementary Schrödinger formalism:

$$A^{(1)} = \sum_{i=1}^{N} \hat{a}(x_i, \tfrac{\partial}{\partial x_i}; \hat{\mathbf{s}}_i) = \sum_i \hat{a}_i \qquad ; \quad \sum_i \hat{a}_i \, \Phi(x_1, s_1, \ldots, x_N, s_N)$$

A_α =eigenvalues, $f_\alpha \equiv$ eigenfunctions

(Bsp) $A^{(1)}$ = total kinetic energy

(Bsp) $A^{(1)}$ = density

(Bsp) $A^{(1)}$ = magnetization = total magnetic moment in $z-$direction per volume $\mathcal{V}$

0.2.2 field operators

convention concerning notation:

ν	...	energy eigenvalue	creation op.:	$a^\dagger_\nu$
$\hbar k$	...	momentum eigenvalue	creation op.:	$c^\dagger_k$
$\mathbf{r}$	...	space eigenvalue	creation op.:	$\psi^\dagger_\mathbf{r}$
α	...	arbitr. eigenvalue	creation op.:	$a^\dagger_\alpha$

2 possibilities to introduce them:

- most generally (bird's eyes view) by defining

  $a^{(\dagger)}_\alpha$ ... (creates)annihilates 1 additional particle in eigenstate f_α of s.p. operator $A^{(1)}$ if possible (and α mat be ν or $\mathbf{k}$ or x or whatsoever), since no representation is superior to any other good for general considerations sometimes, however, one doesn't only want to know things in general but wants to compute an actual quantity:

- start (as we did) with single–particle part of Hamiltonian $\hat{h}_i \to \phi_\nu \;\Rightarrow\;$ MB wave fct $\big|\ldots n_\nu \ldots\rangle$ $\Rightarrow$ creation/annihilation operators $a_\nu^{(\dagger)}$ $\Rightarrow$ define further such operators by the transformation

$$\boxed{\psi_x \;:=\; \sum_\nu \phi_\nu(x) a_\nu} \;=\; \sum_\nu a_\nu \,\langle\nu| \qquad ; \quad \psi_{\mathbf{r}} \;:=\; \frac{1}{\mathcal{V}^{1/2}} \sum_k e^{i\mathbf{k}\cdot\mathbf{r}}\, c_{\mathbf{k}}$$
$$\psi_x^\dagger \;:=\; \sum_\nu \phi_\nu^*(x) a_\nu^\dagger \;=\; \sum_\nu |\nu\rangle\, a_\nu^\dagger$$

then **any** (arbitrary) single–particle property $A^{(1)}$:

$$\begin{array}{llll}
\text{space repr.:} & \boxed{A^{(1)} \;=\; \int dx\, dx'\; \psi_x^\dagger A_{x,x'} \psi_x} & \text{with} & A_{x,x'} \;=\; \hat{a}\big(x, \tfrac{\partial}{\partial x}\big)\, \delta_{x,x'} \\
\text{energy repr.:} & \boxed{A^{(1)} \;=\; \sum_{\nu,\nu'} a_\nu^\dagger A_{\nu,\nu'} a_{\nu'}} & \text{with} & A_{\nu,\nu'} \;=\; \langle\nu|\hat{a}|\nu'\rangle \;=\; \int dx\; \phi_\nu^*(x)\, \hat{a}\big(x, \tfrac{\partial}{\partial x}\big)\, \phi_{\nu'}(x) \\
\text{momentumrepr.:} & \boxed{A^{(1)} \;=\; \sum_{\nu,\nu'} c_{\mathbf{k}}^\dagger A_{\mathbf{k},\mathbf{k}'} c_{\mathbf{k}'}} & \text{with} & A_{\mathbf{k},\mathbf{k}'} \;=\; \langle\mathbf{k}|\hat{a}|\mathbf{k}'\rangle \;=\; \ldots \\
\text{arbitrary:} & \boxed{A^{(1)} \;=\; \sum_{\alpha,\alpha'} a_\alpha^\dagger A_{\alpha,\alpha'} a_{\alpha'}} & \text{with} & \ldots
\end{array} \tag{4}$$

proof: one of them VL ,,Höhere Quantentheorie", the other → homework

(Bem) change between different observables $\widehat{=}$ unitary transformation → homework

why are they called ,,single–particle" properties? cf. later in this section
first some examples:

(Bsp) single particle Hamiltonian

(Bsp) (total) momentum

(Bsp) density: $A^{(1)} = \rho(\mathbf{r})$ ($\mathbf{r}$ = free variable → use $\mathbf{r}', \mathbf{r}''$ in matrix repr.)

$\mathbf{r} \to \mathbf{k} \to$ homework

$$\boxed{\hat{\rho}(\mathbf{r}) = \psi_{\mathbf{r}}^\dagger\, \psi_{\mathbf{r}}} \qquad \boxed{\hat{\rho}(\mathbf{q}) = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}+\mathbf{q}}}$$

(convention for F.T.: $\tilde{f}(\mathbf{q}) = \int d^3r\; e^{-i\mathbf{r}\cdot\mathbf{q}} f(\mathbf{r})$; $f(\mathbf{r}) = \frac{1}{\mathcal{V}} \int d^3q\; e^{+i\mathbf{r}\cdot\mathbf{q}} \tilde{f}(\mathbf{q})$)

Bsp ,,s.p. Hamiltonian part" of Dirac's perturbation operator:

$H = \widetilde{H}^0 + V + U^{\text{ext}}$ then $S = T\, e^{\int dt'\, [V + U^{\text{ext}}]}$

↑ Einsteinkonvention → $\boxed{S = T\, e^{\psi^\dagger_{\mathbf{r}}\, U^{\text{ext}}_{\mathbf{r}\mathbf{r}'}\, \psi_{\mathbf{r}'}}}$

Here, T is the time ordering operator. We'll deal with time later, now just accept that we work in Heisenberg representation and all operators carry the corresponding time dependence.

why are the $A^{(1)}$ called ,,single–particle" properties?
because there must be at least 1 particle present in the system in order that $A^{(1)}$ is observable ($\neq 0$).
let's check this:

Bsp $A^{(1)}$ acting on Φ_{V}

Bsp $A^{(1)}$ acting on Φ_μ

$\langle \Phi_\mu | A^{(1)} | \Phi_\mu \rangle$

$A^{(1)}$ acting on $\Phi^{(1)}$

Bsp $A^{(1)}$ acting on Φ_{μ_1,μ_2}

$\langle \Phi_{\mu_1,\mu_2} | A^{(1)} | \Phi_{\mu_1,\mu_2} \rangle$

$\langle \Phi_0 | A^{(1)} | \Phi_0 \rangle$

Bem $A^{(1)}\, \Phi_{\mathbf{r}_1,\mathbf{r}_2} \;\Rightarrow\;$ Schröd.darstellung

0.2.3 Spin

sometimes spelled out explicitly; here: most of the time „swallowed" in α, e.g. $\nu = (n, \sigma)$, $k = (\mathbf{k}, \sigma)$, $x = (\mathbf{r}, \sigma)$, and $\int dx \equiv \sum_\sigma \int d^3r$ etc.

then: $A^{(1)} = \sum_{\alpha,\alpha'} \ldots \widehat{=} \sum_{\sigma,\sigma'} \sum_{\mathbf{k},\mathbf{k}'} a^\dagger_{\mathbf{k},\sigma} A_{\substack{\mathbf{k}\mathbf{k}'\\ \sigma\sigma'}} a_{\mathbf{k}'\sigma'}$ with $A_{\substack{\mathbf{k}\mathbf{k}'\\ \sigma\sigma'}} = \int dx\, \phi^*_{\mathbf{k},\sigma}(x)\, \hat{a}(x, \frac{\partial}{\partial x}, \hat{\mathbf{s}})\, \phi_{\mathbf{k}'\sigma'}(x)$

transformation to real space: in most cases (and in all cases considered in this lecture) spin and space are separated: $\phi_k = \phi_{\mathbf{k},\sigma} = \varphi_{\mathbf{k}} \eta_\sigma$

$$\psi_x = \sum_k \phi_k(x) c_k \quad \rightarrow \begin{cases} \text{either} & \psi_{\mathbf{r}} = \sum_{\mathbf{k},\sigma} \phi_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \\ \text{or} & \psi_{\mathbf{r},\sigma} = \sum_{\mathbf{k}} \varphi_{\mathbf{k}} c_{\mathbf{k},\sigma} \end{cases}$$

Both possibilities can be found in the literature; I prefer the lower point of view.
Here η_σ = EF of $\underline{\underline{\sigma_z}}$ Pauli spin matrx $\Rightarrow$ use this representation for $\hat{\mathbf{s}}$:

$$\eta_\sigma \cdot \hat{\mathbf{s}} \cdot \eta'_\sigma = g\mu_{\mathrm{B}} \tfrac{\hbar}{2} \underline{\underline{\vec{\sigma}}}_{\sigma\sigma'} \qquad \text{or} \qquad \eta_\sigma \cdot 1 \cdot \eta'_\sigma = \delta_{\sigma\sigma'}$$

then general $A^{(1)} = \int dx\, dx'\, \psi^\dagger_x A_{x,x'} \psi_x = \sum_{\sigma,\sigma'} \int d^3r d^3r'\, \psi^\dagger_{\mathbf{r},\sigma} A_{\substack{\mathbf{r}\mathbf{r}'\\ \sigma\sigma'}} \psi_{\mathbf{r}',\sigma'}$ with $A_{\substack{\mathbf{r}\mathbf{r}'\\ \sigma\sigma'}} = \hat{a}\big(\mathbf{r}, \frac{\partial}{\partial \mathbf{r}}\big)_{\sigma,\sigma'} \delta_{\mathbf{r},\mathbf{r}'}$

and $\hat{a}(\ldots)_{\sigma,\sigma'}$ from Pauli matrices

(Bsp) density

(Bsp) total magnetic moment / magnetization

$$\mathbf{M} = \sum_i \hat{\mathbf{s}}_{zi} \quad \text{with} \quad \hat{\mathbf{s}}_z = \tfrac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

combine the 2: $\boxed{\mathcal{M}(\mathbf{r}) = \psi^\dagger_{\mathbf{r}\uparrow} \psi_{\mathbf{r}\uparrow} - \psi^\dagger_{\mathbf{r}\downarrow} \psi_{\mathbf{r}\downarrow}}$

(Bsp) magnetization in $x-$direction (if some ext magnetic field defines the $z-$direction) $\rightarrow$ homework

0.2.4 pair properties

Elementary Schrödinger picture: $A^{(2)} = \sum_{i\neq j} \hat{a}\big(x_1, \frac{\partial}{\partial x_1}, x_2, \frac{\partial}{\partial x_2}, \big)$

Without further proof, in analogy to $A^{(1)} = \sum_{\alpha,\alpha'} a^\dagger_\alpha A_{\alpha,\alpha'} a_{\alpha'}$ now

$$\text{space repr.:} \quad \boxed{A^{(2)} = \int dx_1 dx_2\, dx_2' dx_1'\; \psi^\dagger_{x_1} \psi^\dagger_{x_2}\, A_{x_1 x_2 x_2' x_1'}\, \psi_{x_2'}\, \psi_{x_1'}} \quad \text{with} \quad \hat{a}\big(x_1, \tfrac{\partial}{\partial x_1}, x_2, \tfrac{\partial}{\partial x_2}, \big)\, \delta_{x_1,x_1'} \delta_{x_2,x_2'}$$

$$\text{arbitrary:} \quad \boxed{A^{(2)} = \sum_{\alpha_1 \ldots \alpha_2'} a^\dagger_{\alpha_1}\, a^\dagger_{\alpha_2}\, A_{\alpha_1 \alpha_2 \alpha_2' \alpha_1'}\, a_{\alpha_2'}\, a_{\alpha_1'}} \quad \text{with} \quad \langle \alpha_1 \alpha_2 | \hat{a} | \alpha_1' \alpha_2' \rangle \tag{5}$$

(proof: VL „Höhere Quantentheorie" or accept it as analogy)

general remarks:

- 1–particle propts contain 1 a and 1 $a^\dagger$
  2–particle propts contain 2 a and 2 $a^\dagger$
  ...
  N–particle propts contain N a and N $a^\dagger$

- of course, there may also be physical propts, or at least operators containing different numbers of $a-$ and $a^\dagger-$ operators. Such quantities do not commute with the particle number:

$$N = \int dx\; \psi^\dagger_x \psi_x = \sum_\nu a^\dagger_\nu a_\nu = \sum_k c^\dagger_k c_k = \ldots\ldots$$

  (proof that $\big[A^{(n)}, N\big]_- = 0 \rightarrow$ homework). They become interesting, when N is not conserved (e.g. cooper pairs); (not for us).

- $A^{(2)}\Phi_{\rm V} = 0\,, \quad A^{(2)}\Phi^{(1)} = 0\,, \quad A^{(2)}\Phi^{(2)} \neq 0\,, \quad A^{(2)}\Phi^{(3)} \neq 0\,, \quad \ldots$
  (i.e. at least 2 particles necessary to observe this property)

specific properties:

- **interaction** V: $\frac{1}{2}\sum_{i<j} v(\mathbf{r}_i, \mathbf{r}_j)$

$$\boxed{V = \frac{1}{2}\int dx_1 dx_2\; \psi^\dagger_{x_1} \psi^\dagger_{x_2}\;\; v(\mathbf{r}_{12})\, \psi_{x_2} \psi_{x_1}} = \frac{1}{2}\sum_{\sigma,\sigma'} \int d^3r d^3r'\; \psi^\dagger_{\mathbf{r}\sigma} \psi^\dagger_{\mathbf{r}'\sigma'}\, v(\mathbf{r}-\mathbf{r}')\, \psi_{\mathbf{r}'\sigma'} \psi_{\mathbf{r}\sigma}$$

  if the F.T. of v exists (spin suppressed) $\longrightarrow$ homework

$$V = \frac{1}{2}\frac{1}{\mathcal{V}} \sum_{\mathbf{q}} \widetilde{v}(q) \sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}}\, c^\dagger_{\mathbf{k}'} c_{\mathbf{k}'+\mathbf{q}} c_{\mathbf{k}\,-\mathbf{q}}$$

- **pair density** $\rho^{(2)}$:
  recall: $\rho(\mathbf{r}) = N \int d^3r_2 \ldots d^3r_N\, |\Phi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2 \;\;\widehat{=}\;\; \hat{\rho} = \sum_i \delta(\mathbf{r}-\mathbf{r}_i) \;\;\widehat{=}\;\; \hat{\rho} = \psi^\dagger_{\mathbf{r}} \psi_{\mathbf{r}}$
  $\rho^{(2)}(\mathbf{r}, \mathbf{r}') = N(N-1) \int d^3r_3 \ldots d^3r_N\, |\Phi(\mathbf{r}, \mathbf{r}', \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2 \;\;\widehat{=}\;\; \hat{\rho}^{(2)} = \sum_{i\neq j} \delta(\mathbf{r}-\mathbf{r}_i)\delta(\mathbf{r}'-\mathbf{r}_j)$

$$\boxed{\hat{\rho}^{(2)} = \psi^\dagger_x\, \psi^\dagger_{x'} \psi_{x'} \psi_x} \;\; \longrightarrow \;\; \begin{array}{ll} \hat{\rho}^{(2)}(\mathbf{r}, \mathbf{r}') = \sum_{\sigma,\sigma'} \psi^\dagger_{\mathbf{r}\sigma}\; \psi^\dagger_{\mathbf{r}'\sigma'} \psi_{\mathbf{r}'\sigma'} \psi_{\mathbf{r}\sigma} & \text{spacial pair density} \\ \hat{\rho}^{(2)}(\mathbf{r}, \sigma, \mathbf{r}'\sigma') = \psi^\dagger_{\mathbf{r}\sigma}\; \psi^\dagger_{\mathbf{r}'\sigma'} \psi_{\mathbf{r}'\sigma'} \psi_{\mathbf{r}\sigma} & \text{spin dep. pair dens.} \end{array}$$

thus $V = \frac{1}{2}\int d^3r_1 d^3r_2\, v(\mathbf{r}_{12})\, \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$

corresponding expectation values:

density: $\langle\hat\rho(\mathbf{r})\rangle \xrightarrow[\text{homog.system}]{} \frac{N}{\mathcal{V}} =: n$

pair density: $\langle\hat\rho^{(2)}(\mathbf{r},\mathbf{r}')\rangle \xrightarrow[\text{homog.system}]{} \boxed{\rho^{(2)}(|\mathbf{r}-\mathbf{r}'|) \;=:\; n^2\, g(|\mathbf{r}-\mathbf{r}'|)}$

pair distribution function

(in inhom systems: $\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2) =: \rho^{(1)}(\mathbf{r}_1)\rho^{(1)}(\mathbf{r}_2)g(\mathbf{r}_1,\mathbf{r}_2)$)

physical meaning: correlation

normalization: $\int d^3r d^3r'\, \rho^{(2)} = N(N-1) \quad\Rightarrow\quad \int\frac{d^3r}{\mathcal{V}}\, g(r) = 1 - \frac{1}{N}$

asymptotics: $\rho^{(2)} \to \rho^{(1)}\rho^{(1)} \quad\Rightarrow\quad g(r\to\infty) \to 1$

static structure factor:

commutation relation: $\psi^\dagger_{x'}\psi_x = \delta_{x,x'} - \psi_x\, \psi^\dagger_{x'} \quad\Rightarrow$

$$\hat\rho^{(2)}_{x,x'} \;=\; \delta_{x,x'}\hat\rho_x + \hat\rho_x\,\hat\rho_{x'} \qquad ; \qquad n^2\, g(r_{12}) \;=\; n\,\delta(\mathbf{r}_{12}) + \langle\hat\rho(\mathbf{r}_1)\hat\rho(\mathbf{r}_2)\rangle$$

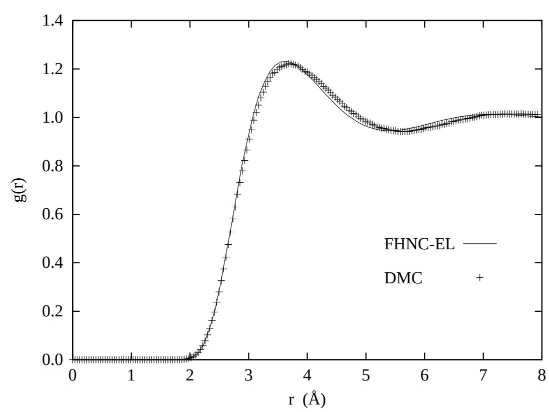
split off n: $\boxed{\delta\hat\rho := \hat\rho - \langle\hat\rho\rangle} = \hat\rho - n$ (for hom.systems)

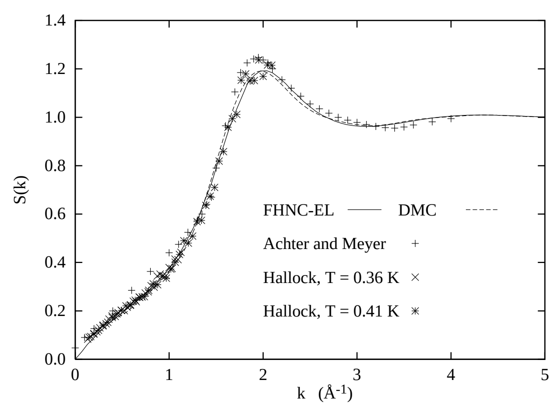
define:

$$\boxed{n\, S(r_{12}) \;:=\; \langle\delta\hat\rho_{\mathbf{r}_1}\delta\hat\rho_{\mathbf{r}_2}\rangle} \qquad n\, S(\mathbf{r}) \;:=\; \int\frac{d^3r'}{\mathcal{V}}\,\langle\delta\hat\rho_{\mathbf{r}+\mathbf{r}'}\,\delta\hat\rho_{\mathbf{r}'}\rangle$$

$$n\,[g(r_{12}) - 1] \;=\; S(r_{12}) + \delta(\mathbf{r}_{12}) \qquad\Leftrightarrow\qquad \boxed{n\,[g(r_{12} - 1] \;=\; \text{F.T.}[S(q) - 1]}$$

$S(q)\ldots$directly **measurable** via scattering experiments!





comparison MC simulation (Casulleras, Boronat (00)) ↔ ,,FHNC/EL" theory (kro (00))
↔ experiment (Achter+Meyer (69), Hallock (72)) (from: kro ,,polish" (2000))

0.2.5 some more remarks

is $S(q)$ a ,,single–particle" or a ,,two–particle=pair" property?

a pair property, but not a ,,pure" one

Dirac's perturbation operator:
$H = \widetilde{H}^0 + V + U^{\mathrm{ext}}$ and $S = T\, e^{\int dt'\, [V + U^{\mathrm{ext}}]}$ (with T = time ordering operator)

again Einsteinkonvention; and $\underline{\mathbf{1}} \equiv \mathbf{r}_1, \sigma_1$ $\boxed{S = T\, e^{\psi^\dagger_{\underline{\mathbf{1}}}\, U^{\mathrm{ext}}_{\underline{\mathbf{11'}}} \psi_{\underline{\mathbf{1'}}} + \frac{1}{2}\psi^\dagger_{\underline{\mathbf{1}}}\, \psi^\dagger_{\underline{\mathbf{2}}}\, V_{\underline{\mathbf{122'1'}}} \psi_{\underline{\mathbf{2'}}} \psi_{\underline{\mathbf{1'}}}}}$
(include also $\int dt'$ in sum.convention) (contains $A^{(n)}$ up to arbitrarily high n)

Calculation of ground state energy:

$$E = \langle H \rangle = \langle \widetilde{H}^0 + U^{\mathrm{ext}} + V \rangle = \langle H^{(1)} + V^{(2)} \rangle$$

$$= \int dx dx'\, h^{(1)}_{xx'}\, \langle \psi^\dagger_x\, \psi_{x'} \rangle + \tfrac{1}{2} \int dx_1 dx_2\, v(r_{12})\, \langle \psi^\dagger_{x_1}\, \psi^\dagger_{x_2}\, \psi_{x_2}\, \psi_{x_1} \rangle$$

$$\downarrow \qquad\qquad\qquad \downarrow$$

$$\equiv \rho^{(1)}_{xx'} \qquad\qquad\qquad = \rho^{(2)}_{x_1 x_2}$$

(single part.) density matrix pair density

For most properties it is not necessary to know the wave function / the state vector, the knowledge of $\rho^{(1)}_{xx'}$ and $\rho^{(2)}_{x_1x_2}$ is sufficient. $\longrightarrow$ look for ways to compute those directly!
Hohenberg Kohn theorem: $E = E[\rho(\mathbf{r})]$, i.e. for the energy even less functions are required!

0.3 Time

0.3.1 Heisenberg Representation

Schrödinger picture:	state vectors	Φ	time–dependent	$-\frac{\hbar}{i}\frac{\partial}{\partial t}\,\Phi = H\Phi$
	properties	A	time–independent	
Heisenberg picture:	state vectors	Φ	time–independent	
	properties	A	time–dependent	$-\frac{\hbar}{i}\frac{\partial}{\partial t}\,A = \big[A, H\big]$

each $A \;=\; e^{+\frac{i}{\hbar}H\,t}\,A\,e^{-\frac{i}{\hbar}H\,t} \quad\longleftrightarrow\quad$ each $a^{(\dagger)} \;=\; e^{+\frac{i}{\hbar}H\,t}\,a^{(\dagger)}\,e^{-\frac{i}{\hbar}H\,t}$

(Bsp) free System $a_\nu(t)$

byproduct: $f(H)\,a$

(Bsp) interacting system: equation of motion (EOM) for ψ_x

in momentum space: EOM for c_k: $\rightarrow$ homework

1 Single Particle Propagator

1.0 Definition of the Propagators

1.0.1 Multiple Times and Time Ordering

formal motivation: Dirac's perturbation operator:

give every operator its own time: $\boxed{\psi_{x_1,t} \longrightarrow \psi_{x_1,t_1} \equiv \psi_1}$

$\int dx_1 \longrightarrow \int dt_1 \int dx_1 \sum_{\sigma_1} \equiv \int d1$

these guys are still supposed to describe the same properties discussed so far:
$A_t^{(1)}$:

$A_t^{(2)}$:

caution: $[\psi_1^\dagger, \psi_2] \neq \delta x_1, x_2$! commut.relations only hold for equal times!

time ordering operator:

Def Geg seien 2 Operatoren B_{t_1} und B_{t_2}. $\boxed{T\, B_{t_1}\, B_{t_2} \;:=\; \theta(t_{12})\, B_{t_1}\, B_{t_2} \mp \theta(t_{21})\, B_{t_2}\, B_{t_1}}$

VZ: $-$ ... Fermioperatoren
$+$ ... Boseoperatoren

$$T\, B_{t_2}\, B_{t_1} \;=\;=\; \mp T\, B_{t_1}\, B_{t_2}$$

now:
$T\, A^{(1)}$

$T\, A^{(2)}$

$$T\, A^{(n)} = A^{(n)}$$

Thus: $A = T\,A$ and $T\,B_2\,B_1 = -T\,B_1\,B_2 \;\Rightarrow$ we now may anticommute the $\psi^\dagger$, ψ in the A as we like, in particular

$$\langle A^{(1)}\rangle \;=\; \langle T\, A^{(1)}\rangle \;=\; \langle \int d1d1'\, A_{11'} T\left(\psi_1^\dagger\, \psi_{1'} \rightarrow -\psi_{1'}\psi_1^\dagger\right)\rangle \;=\; -\int d1d1'\, A_{11'}\, \langle T\, \psi_{1'}\psi_1^\dagger\, \rangle$$

Def $i\hbar g^{(1)} = \boxed{i\, g_{1'1} \;:=\; \langle T\, \psi_{1'}\psi_1^\dagger\, \rangle}$ **single particle propagator**

$i\hbar g^{(2)} = \; i\, g_{1'2'21} \;:=\; \langle T\, \psi_{1'}\psi_{2'}\psi_2^\dagger\, \psi_1^\dagger\, \rangle$ pair propagator

$i\hbar g^{(n)} = \;\ldots$ $n-$particle propagator

Then (with Einstein convention)

$\boxed{\langle A^{(1)}\rangle \;=\; -i\hbar\, A_{11'}\, g_{1'1} = -i\hbar\, \mathrm{Tr} A g}$; $\langle A^{(2)}\rangle \;=\; +i\hbar\, A_{122'1'}\, g_{1'2'21} = +i\hbar\, \mathrm{Tr} A^{(2)} g^{(2)}$

$$\langle A^{(n)}\rangle \;=\; \ldots \;=\; (-1)^n\, i\hbar\, \mathrm{Tr} A^{(n)} g^{(n)}$$

1.1 Single particle propagator: general properties

energy

in particular: expectation value of $A = H$:

$$E \;=\; \langle H\rangle \;=\; \langle H^{(1)} + V^{(2)}\rangle \;=\; -i\hbar\,\mathrm{Tr}\,H^{(1)}g^{(1)} + \frac{1}{2}i\hbar\,\mathrm{Tr}\,V^{(2)}g^{(2)}$$

another dirty trick of the same type:
$\dot{\psi}_{x,t} \;\longrightarrow\; \frac{\partial}{\partial t_1'}\psi_{\underline{1}',t_1'} \;=\; ... + \int d\underline{2}\; v_{\underline{1}'\underline{2}}\psi^\dagger_{\underline{2}}\psi_{\underline{2}}\,\psi_{\underline{1}',t_1'}$ insert appropriate $\delta-$fcts (be careful with δ_{t_1',t_1})
compare with explicit expression for $\mathrm{Tr}\,V^{(2)}g^{(2)}$ $\Rightarrow$

$$E \;=\; -\frac{i\hbar}{2}\,\mathrm{Tr}\left[H^{(1)} - \frac{\hbar}{i}\frac{\partial}{\partial t_1}\right]g^{(1)}$$

$\Rightarrow$ single-particle propagator yields ,,all" we want! (energy $\rightarrow$ same way $\rho^{(2)} \rightarrow g$, S, that's already a lot),
this is the advantage of multiple-time usage.

physical content of the $g^{(1)}$ function:

$\lvert\Phi\rangle$	...	exact (not $V=0$!) $N-$particle (ground) state
$\psi_1^\dagger\,\lvert\Phi\rangle$	...	at $t=t_1$ create an additional particle in $\mathbf{r}_1$ with spin σ_1
$\psi_{1'}\psi_1^\dagger\,\lvert\Phi\rangle$	...	at $t=t_1'$ destroy one particle in $\mathbf{r}_1'$ with spin σ_1'
$\langle\Phi\,\lvert\psi_{1'}\psi_1^\dagger\,\rvert\Phi\rangle$	...	compare with the original state
$\theta_{t_{1'1}}\,\langle\Phi\,\lvert\psi_{1'}\psi_1^\dagger\,\rvert\Phi\rangle$	...	do this at a time t_1' later than t_1

$\lvert\Phi\rangle$	...	$N-$particle (ground) state
$\psi_{1'}\,\lvert\Phi\rangle$	...	at $t=t_1'$ destroy one of the particles in $\mathbf{r}_1'$ with spin σ_1'
$\psi_1^\dagger\,\psi_{1'}\,\lvert\Phi\rangle$	...	at $t=t_1$ create a particle in $\mathbf{r}_1$ with spin σ_1
$\langle\Phi\,\lvert\psi_1^\dagger\,\psi_{1'}\,\rvert\Phi\rangle$	...	compare with the original state
$\theta_{t_{11'}}\,\langle\Phi\,\lvert\psi_1^\dagger\,\psi_{1'}\,\rvert\Phi\rangle$	...	do this at a time t_1 later than t_1'

$g^{(1)}$ in homogeneous systems:

clearly, $i\hbar g^{(1)} = \langle T\psi_1\psi_2^\dagger\rangle \;=\; \propto g(\mathbf{r}_1,\sigma_1,t_1,\,\mathbf{r}_2,\sigma_2,t_2)$

homogeneous system: $(\mathbf{r}_1,\mathbf{r}_2) \;\rightarrow\; |\mathbf{r}_{12}| = r_{12}$

time:

$$\langle\psi_{\underline{1},t_1}\psi^\dagger_{\underline{2},t_2}\rangle \;=\; e^{\frac{i}{\hbar}Et_{12}}\,\langle\psi_{\underline{1}}\,e^{-iHt_{12}}\,\psi^\dagger_{\underline{2}}\rangle \qquad \text{only time difference relevant}$$

$$\boxed{g^{(1)} \;=\; g_{\sigma,\sigma'}(r_{12},t_{12}) \qquad \leftrightarrow \qquad g_{\sigma,\sigma'}(k,\omega)}$$

1.2 Free single particle propagator: g^0

We now calculate $i\hbar g^0(\mathbf{r}_1, \mathbf{r}_2, t_{12}) = \langle T \psi_1 \psi_2^\dagger \rangle_0$ where $\langle \ldots \rangle_0$ is the noninteracting (=free) ground state:

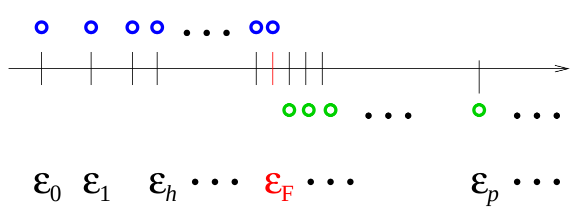
$$\boxed{i\hbar g^0(\mathbf{r}_1, \mathbf{r}_2, t_{12}) \;=\; \sum_\nu \varphi_\nu(\mathbf{r}_1)\varphi_\nu^*(\mathbf{r}_2)\, e^{-\frac{i}{\hbar}\varepsilon_\nu t_{12}} \left[\theta_{t_{12}} n_\nu^- - \theta_{t_{21}} n_\nu\right]}$$

With spin: $\langle a_{\nu'}^\dagger a_{\nu} \rangle_0 \propto \delta_{\sigma\sigma'}$

Fourier transform:
($\rightarrow$ homework: recall FT of $\pm\theta(\pm t)$)

$$\boxed{g^0(\mathbf{r}_1, \mathbf{r}_2, \omega) \;=\; \sum_\nu \varphi_\nu(\mathbf{r}_1)\varphi_\nu^*(\mathbf{r}_2) \left[\frac{n_\nu^-}{\hbar\omega - \varepsilon_\nu + i0^+} + \frac{n_\nu}{\hbar\omega - \varepsilon_\nu - i0^+}\right]}$$

Just remember where the poles are



$$g^0(\mathbf{r}_1, \mathbf{r}_2, \omega) \;=\; \sum_\nu \varphi_\nu(\mathbf{r}_1)\varphi_\nu^*(\mathbf{r}_2) \frac{1}{\hbar\omega - \varepsilon_\nu}$$

Schreibweise kro:

special case: homogeneous system:

Equation of motion ($\equiv$ eom)

eom for $i\hbar g^0$:

$$\boxed{\left(-\frac{\hbar}{i}\frac{\partial}{\partial t_1} - \hat{h}^0_{\underline{1}}\right) g^0_{12} \;=\; \delta_{12}} \qquad \widehat{D}^0\, g^0_{12} \;=\; \delta_{12}$$

typical eom for a GF!! 1−particle Schröd.eq.!

retarded GF

(Def) $i\hbar g^{\text{ret}}_{12} \;:=\; \theta(t_{12})\left[\langle\psi_1\psi_2^\dagger\rangle + \langle\psi_2^\dagger\psi_1\rangle\right]$

eom

obeys same differential equation!

Fourier Transform $t \longrightarrow \omega$:

$$ig^{0\text{ ret}}(\mathbf{r}_1, \mathbf{r}_2, \omega) \;=\; \sum_\nu \varphi_\nu(\mathbf{r}_1)\varphi^*_\nu(\mathbf{r}_2)\,\frac{1}{\hbar\omega - \varepsilon_\nu + i0^+}$$

avanced GF

analogously, same eom, all $\omega \;\rightarrow\; \omega - i0^+$

time-ordered, ret and av GF all same diff.eq., different poles in komplex ω−plane

the way back

Ideology: $g^{(1)}$ = powerful $\rightarrow$ calculate ,,somehow" $g^{(1)}(.,.,\omega)$ $\rightarrow$ now calculate $A^{(1)}$ from this

$A^{(1)} =$

$$A^{(1)} = \int d\underline{1}d\underline{1}'\, \hat{a}\delta_{\underline{1}\underline{1}'} \int \frac{d\omega}{2\pi i}\, e^{+i\omega 0^+}\, g^{(1)}(\mathbf{r}_{\underline{1}}, \mathbf{r}_{\underline{1}'}, \omega)$$

e.g. particle density:

1.3 Single particle propagator $g^{(1)}$: exact relations

1.3.1 Non-interacting equation of motion

$$\boxed{g_{12} = g^0_{12} + g^0_{13}\, U^{\text{ext}}_{34}\, g_{42}}$$

Diagrams:

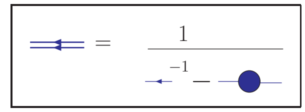
successive isertion:

solve for g

$$\boxed{g_{12} = \begin{cases} \left([\delta - g^0 U]^{-1}\right)_{13} g^0_{32} & = [\delta - g^0 U]^{-1}\, g^0 \\ g^0_{13}\left([\delta - U g^0]^{-1}\right)_{32} & = g^0\,[\delta - U g^0]^{-1} \end{cases}}$$

in diagrams

pull out g^0 on the other side:



Spin:
Cf. derivation of $g^0(\underline{1}, \underline{2}, t_{12})$: contains $\langle a_\nu \, a^\dagger_{\nu'} \rangle \;\rightarrow\; \delta_{\nu,\nu'}$ etc, thus

$$g^0(\underline{1}, \underline{2}, t_{12}) \;\propto\; \delta_{\sigma_1,\sigma_2} \qquad ; \qquad g^0(\mathbf{r}_1, \mathbf{r}_2, t_{12}) \;:=\; \sum_{\sigma_1,\sigma_2} g^0_{12} \;=\; \sum_{\sigma} \sum_{\nu} \ldots$$

If external potential spin–independent: $u_{34} = u_{\underline{3}} \, \delta_{\underline{34}} \;\propto\; \delta_{\sigma_3,\sigma_4} \quad \Rightarrow\; g^{(1)} \;\propto\; \delta_{\sigma_1,\sigma_2}$

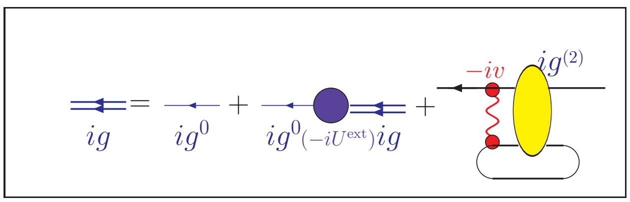
1.3.2 Interacting equation of motion

Start again with $-\frac{\hbar}{i}\frac{\partial}{\partial t_1}\, g_{12} \;=\; \delta_{12} \;+\; \langle \left(-\frac{\hbar}{i}\dot{\psi}_1\right) \psi_2^\dagger \rangle$

thus

$$-\frac{\hbar}{i}\frac{\partial}{\partial t_1}\, g_{12} \;=\; \delta_{12} \;+\; \hat{h}^0_{\underline{1}}\, g_{12} \;+\; U^{\rm ext}_{14}\; g_{42} \;-\; v_{155'6}\; g^{(2)}_{65'52}$$

$$g_{12} \;=\; g^0_{12} \;+\; g^0_{13}\, U^{\rm ext}_{34}\; g_{42} \;-\; g^0_{13}\, v_{355'4}\; g^{(2)}_{45'52}$$



(-) closed loop

hierarchy!! (eom for $g^{(1)}$ contains $g^{(1)}$; eom for $g^{(2)}$ contains $g^{(3)}$, … etc)
How should one end this? $\rightarrow$ approximations, cf. Sec.[1.3.4] „closure relation"

Before further dealing with equs determining $g^{(1)}$ let's list another exact property:

1.3.3 Lehman representation

recall:

$$g \propto \langle T\psi\psi^\dagger\rangle \;=\; \theta\,\langle\psi\psi^\dagger\rangle \;-\; \theta_-\,\langle\psi^\dagger\psi\rangle \qquad \leftarrow \text{ contains intermediate state(s) with } N\pm 1 \text{ particles}$$

$$g^0 \;=\; \sum_\nu \varphi_\nu(\underline{1})\varphi^*_\nu(\underline{2})\left\{\frac{n^-_\nu}{\hbar\omega-\varepsilon_\nu+i0^+}+\frac{n_\nu}{\hbar\omega-\varepsilon_\nu-i0^+}\right\} \qquad \leftarrow \; N\pm 1 \text{ states have their poles } {}^{\text{below}}_{\text{above}} \text{ the real axis}$$

Without further proof (see, eg., Fetter/Walecka,Inkson or Friedrich/Schindlmayer)

$$g(\underline{1},\underline{2},\,\omega) \;=\; \sum_n\left\{\frac{\phi_n^{N+1}(\underline{1})\phi_n^{*\,N+1}(\underline{2})}{\hbar\omega-\Delta\varepsilon_n^{N+1}+i0^+}+\frac{\phi_n^{N-1}(\underline{1})\phi_n^{*\,N-1}(\underline{2})}{\hbar\omega-\Delta\varepsilon_n^{N-1}-i0^+}\right\}$$

here: numerator

$\Phi_{\mathrm{G}} \;=\; \Phi_0^N$	…	$N-$particle ground state	of the interacting System
Φ_n^N	…	$N-$particle exicited state	of the interacting System
$\psi^\dagger_{\underline{2}}\Phi_n^N$	…	$(N+1)-$particle excited state	…interacting…
$\langle\Phi_0^{N+1}\vert\psi^\dagger_{\underline{2}}\vert\Phi_n^N\rangle$	…	comparison:	$=: \phi_n^{*\,N+1}(\underline{2})$
$\psi_{\underline{1}}\Phi_n^N$	…	$(N-1)-$particle excited state	…interacting…
$\langle\Phi_0^{N-1}\vert\psi_{\underline{1}}\vert\Phi_n^N\rangle$	…	comparison:	$=: \phi_n^{N-1}(\underline{1})$

denominator:

$$\Delta\varepsilon_n^{N\pm1}\ldots \text{ excitation energies } = E_n^{N\pm1}-E_0^N = E_n^{N\pm1}-E_0^{N\pm1} + E_0^{N\pm1}-E_0^N = \varepsilon_n^{N\pm1}+\mu$$

$$\Rightarrow \qquad \boxed{\text{exact } g^{(1)} \text{ has poles at } \omega=\mu+\varepsilon_n^{N\pm1}\mp i0^+ = \begin{cases}\mu+\varepsilon_n^{N+1}-i0^+\\ \mu+\varepsilon_n^{N-1}+i0^+\end{cases}}$$

(though we do not know the excitation energies of the fully interacting system (and even less know the numerator!) we do know the pole structure of the fully interacting $g^{(1)}$).
note: only for low lying excitations the $\varepsilon_n^{N\pm1}$ (may) resemble the free excitation energies and can be labeled by the same qu-numbers ν

1.3.4 Self energy Σ

Starting point: eom for $g^{(1)}$ $\rightarrow$ contains $g^{(2)}$; just leave it away?

$-i\,\mathrm{Tr}1 g^{(1)} \;=$

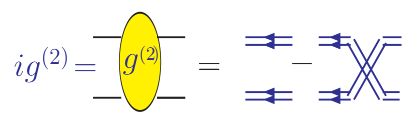
$+i\,\mathrm{Tr}1 g^{(2)} \;=$

$$\text{thus}\quad |\mathrm{Tr} g^{(2)}| \propto N^2 \gg N \propto |\mathrm{Tr} g^{(1)}|$$

$\rightarrow$ one can't just neglect it!

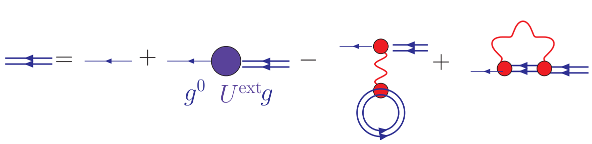
Recall: $\langle \psi^\dagger \psi^\dagger \psi \psi \rangle = \rho^{(2)} \;=\; \rho^{(1)} \rho^{(1)}\, g \quad \Rightarrow \quad$ next try: $\;ig^{(2)} \;=\; ig^{(1)}\, ig^{(1)}$

Symmetry: $\langle \psi_1^\dagger\, \psi_2^\dagger\, \psi_{2'} \psi_{1'} \rangle \;=\; \begin{cases} -\langle \psi_2^\dagger\, \psi_1^\dagger\, \psi_{2'} \psi_{1'} \rangle \\ -\langle \psi_1^\dagger\, \psi_2^\dagger\, \psi_{1'} \psi_{2'} \rangle \end{cases}$

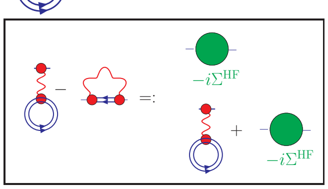


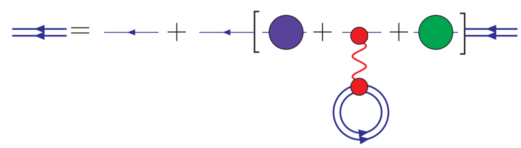
check norm:

then in eom



already soved! (same structure as eom with U)





$$g \;=\; g^0 + g^0 \big[\, U^{\mathrm{ext}} + (.) + \Sigma^{\mathrm{HF}} \,\big]\, g$$

$$\Rightarrow \quad g \;=\; \big[\, 1 + \big(U^{\mathrm{ext}} + (.) + \Sigma^{\mathrm{HF}}\big) g^0 \,\big]^{(-1)} g^0 \;=\; \frac{1}{g^{0\,-1} + U^{\mathrm{ext}} + (.) + \Sigma^{\mathrm{HF}}}$$

A formal way out of the hierarchy problem:

$$\text{redefine} \quad \begin{array}{rcrcr} v\,g^{(2)} = -iv\,ig^{(2)} & =: & -i\Sigma\,ig^{(1)} & = & \Sigma\,g^{(1)} \\ \text{(or)} & =: \; -iv\,ig^{(1)}ig^{(1)} + & -i\Sigma\,ig^{(1)} & = & U_{\mathrm{H}}\,g^{(1)} + \;\Sigma\,g^{(1)} \end{array}$$

eom as above with $\Sigma^{\mathrm{HF}} \to \Sigma$

$\rightarrow$ now look for an equation for Σ

before doing this: have a close look at Σ^{HF}

1.3.5 Hartree–Fock

1.4 Quasi-particles

1.4.1 Formal points of view

So far we have found: $(\hbar \equiv 1)$

free $\quad g^0(\underline{1},\underline{2},\omega) = \sum_\nu \varphi_\nu(\underline{1})\varphi^*_\nu(\underline{2}) \left\{ \frac{n^{0-}_\nu}{\omega-\varepsilon_\nu+i0^+} + \frac{n^0_\nu}{\omega-\varepsilon_\nu-i0^+} \right\} \quad = \mathcal{P}\ldots \pm i\pi\,\delta(\omega-\varepsilon_\nu)$

Lehmann $\quad g(\underline{1},\underline{2},\omega) \;=\; \sum_n \left\{ \frac{\ldots}{\omega-\Delta\varepsilon^{N+1}_n+i0^+} + \frac{\ldots}{\hbar\omega-\Delta\varepsilon^{N-1}_n-i0^+} \right\}$

$\Sigma \quad g^{-1}(\underline{1},\underline{2},\omega) \;=\; (g^0)^{-1}(\underline{1},\underline{2},\omega) - \Sigma(\underline{1},\underline{2},\omega) \qquad$ poles: $\;(g^0)^{-1}-\Sigma=0$

note:

- recall $\varepsilon^{N\pm1}_n$: excitation energies of the *interacting* system, can be *very* different from the ε_ν
- for low lying excitations they *may* resemble the free energies & can be labeled with the same qu-numbers (Landau): $\varepsilon^{N\pm1}_n \to\approx \widetilde{\varepsilon}_\nu$
- these will have a different strength: $(\ldots)\delta$ (as there will be other excitations, e.g. collective modes)
- if we know Σ we can obtain them from $(g^0)^{-1}-\Sigma \;=\; 0$:

  homog. system: $\quad \omega-\varepsilon_k-\Sigma(k,\omega) \;=\; 0 \quad \xleftarrow[\text{solution depends on } k]{} \quad \widetilde{\varepsilon}_k$ qu-particle energies

spectral representation:

Lehmann: $\sum_n \frac{A_n}{\omega-\Delta\varepsilon_n} = \sum_n \int d\omega' \frac{A_n}{\omega-\omega'}\,\delta(\omega'-\Delta\varepsilon_n) = \int \frac{1}{\omega-\omega'}\,\sum_n \ldots =: \int \frac{1}{\omega-\omega'}\,A(\omega')$

(also hink of it that way: $\varepsilon_n 0$ dense lying variable)

$\Delta\varepsilon^{N\pm1}_n = \mu + \varepsilon^{N\pm1}_n \qquad \begin{matrix}\varepsilon^{N+1}_n>0\\ \varepsilon^{N-1}_n<0\end{matrix} \qquad \begin{matrix}\Delta\varepsilon^{N+1}_n>\mu\\ \Delta\varepsilon^{N-1}_n<\mu\end{matrix}$

therefore

$$g(\underline{1},\underline{2},\omega) \;=\; \int_{-\infty}^{\infty} d\omega' \left[\frac{A(\underline{1},\underline{2},\omega')\theta(\omega'-\mu)}{\omega-\omega'+i0^+} + \frac{B(\underline{1},\underline{2},\omega')\theta(\mu-\omega')}{\omega-\omega'-i0^+} \right] \;=\; \int_{-\infty}^{\infty} d\omega'\,\frac{A(\underline{1},\underline{2},\omega')}{\omega-\omega'+i\,\mathrm{sgn}(\omega'-\mu)0^+}$$

$$=\; \int_0^{\infty} d\omega' \left[\frac{\widetilde{A}(\underline{1},\underline{2},\omega')}{\omega-\omega'-\mu+i0^+} + \frac{\widetilde{B}(\underline{1},\underline{2},\omega')}{\omega+\omega'-\mu-i0^+} \right]$$

„spectral densities", „spectral weight functions"
IF $A\approx$ some peak+background $\;\to\;$ „quasiparticle" + bkgr.

1.4.2 physical considerations

cf. Mattuck etc

1.5 Hedin's pentagon

1.5.1 5 Equations

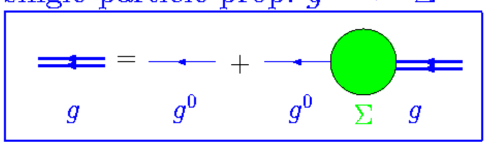
One can show (exactly!, 1965 Hedin) that the many–body problem is characterized by the following 5 quantities obeying the following 5 Equs:

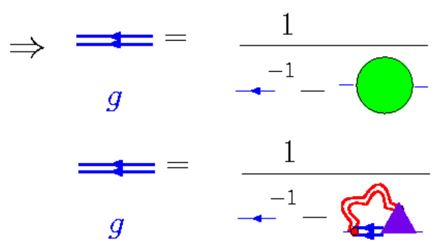
quantities:

$\boxed{g,\ \Sigma,\ W = v^{\text{eff}},\ \Gamma,\ \Pi \mathrel{\widehat{=}} \epsilon}$ represented by diagrams: ig, $-i\Sigma$, $-iW$, Γ, $i\Pi$

equations: (here written for the hom. systems, so $U_{\text{H}} = 0$)

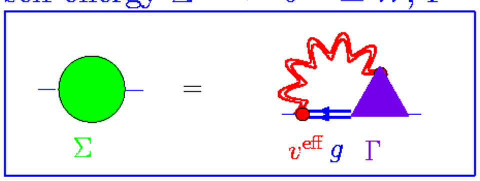
single particle prop. $g \leftarrow \Sigma$



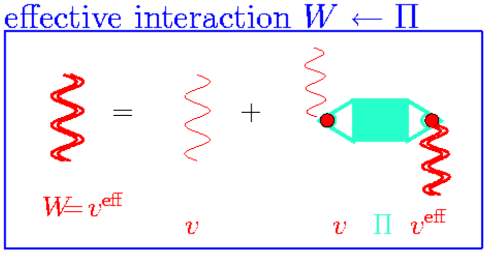


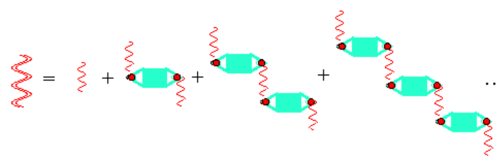
$g = g\,[W, g, \Gamma]$

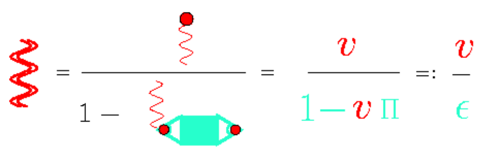
self energy $\Sigma \quad \leftarrow v^{\text{eff}} \equiv W,\, \Gamma$



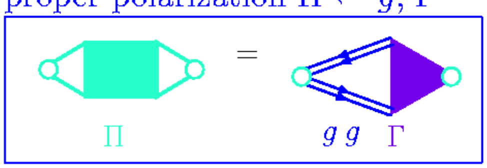
effective interaction $W \leftarrow \Pi$

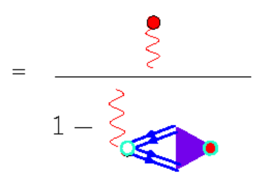






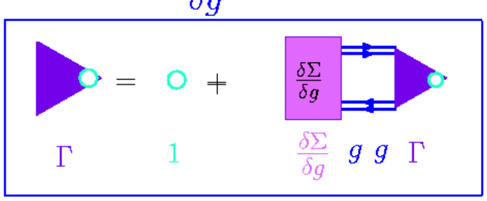
proper polarization $\Pi \leftarrow g,\, \Gamma$





$W = W\,[v, g, \Gamma]$

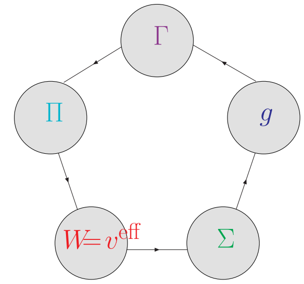
vertex $\Gamma \leftarrow \dfrac{\delta\Sigma}{\delta g}$!!! , Γ



5 eqs, 5 unknowns $\longrightarrow$ looks so solvable :-)

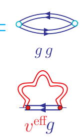
problems: functional drivative!!!, even without: numerically demanding!!!

Ignoring the numerical problems, what would be the strategy?

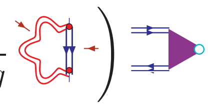


1.a $\Gamma = 1$

1.b $\Pi = g\,g \equiv \widetilde{\Pi}^0\,, \quad W = \dfrac{v}{1 - v\widetilde{\Pi}^0}$

$\widetilde{\Pi}^0 =$ 

1.c $\boxed{\Sigma = g\,W}\,, \quad g = \ldots =: g^{[1]} =: g^{\mathrm{GW}}$

2.a $\Gamma = 1 + \dfrac{\delta\Sigma^{\mathrm{GW}}}{\delta g^{\mathrm{GW}}} g g \Gamma \; = \; 1 + \left(\dfrac{\delta}{\delta g} \right)$  $= \; \ldots$

2.b $\Pi = g\,g\,\Gamma^{[2a]} = \ldots, \quad W = \ldots$

2.c $\Sigma = g\,W\,\Gamma\,, \quad g = \ldots =: g^{[2]} =: g^{\Gamma_2 \mathrm{GW}}$

vertex diagrams in 2a (cf. appendix):

leading correction to Π and Σ:

remarks:

- one can replace the expression with the fct'al derivative by an ∞ series $\quad \to$ homework

- one can reformulate the equs in such a way that not Γ but another one of the 5 quantities is not given in by closed expression

A note on the (numerical) difficulty:

Step „1" of above „GW": We don't know $g \quad \to$ solve selfconsistenly!

1965	Hedin
1969	Hedin-Lundqvist numerical $e-$gas (jellium)
66-75	insulators, semiconductors: static version
~1978	starting from HF, with $\Pi \,\widehat{=}\, \epsilon$ in plasmon-pole-approx.
~1980s	realistic $\Pi \,\widehat{=}\, \epsilon$
~1985s	„ab initio GW" (starting g from DFT orbitals)
2002	Onida/Reining/Rubio: „GW can be considered as the state-of-the-art-tool for band-structure calculations"

(of course, also vertex corrections have been investigated).

1.5.2 Derivation

2 Energy

3 Approximations

2.0 g^0W

2.0.1 ...

Literature (non complete)

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