1.4 From single- to many-particle Green[*] functions

[*] G. Green (1793 – 1841)

Motivation: we want to find a (perturbative) solution of a quantum mechanical system

First we will consider the one-particle Schrödinger equation

$$[H_0(\vec{r}) + V(\vec{r})]\psi_E = E\psi_E \Leftrightarrow [E - H_0]\psi_E = V\psi_E$$

solution known   perturbation (e.g.: scattering problem)

We define a (single-particle) Green function

$$[E - H_0(\vec{r})]\, G_0(\vec{r}, \vec{r}\,', E) = \delta(\vec{r} - \vec{r}\,')$$

analogously to classical electrodynamics

$$\rightarrow G_0^{-1}(\vec{r}, E) = E - H_0(\vec{r}), \quad G_0^{-1}(\vec{r}, E)\, G_0(\vec{r}, \vec{r}\,', E) = \delta(\vec{r} - \vec{r}\,')$$

$$\Rightarrow \boxed{\left[G_0^{-1}(\vec{r}, E) - V(\vec{r})\right]\psi_E = 0}$$

$$\Rightarrow \psi_E(\vec{r}) = \psi_E^0(\vec{r}) + \int d^3r'\, G_0(\vec{r}, \vec{r}\,', E)\, V(\vec{r}\,')\, \psi_E(\vec{r}\,')$$

(inserting into Schrödinger equation gives equality)

→ Solve iteratively

$$\psi_E(\vec{r}) = \psi_E^0(\vec{r}) + \int d^3r'\, G_0(\vec{r}, \vec{r}\,', E)\, V(\vec{r}\,')\, \psi_E^0(\vec{r}\,') + \mathcal{O}(V^2)$$

⇒ G_0 is building block of propagation of unperturbed system time-dependence: $\left[i\partial_t - H_0(\vec{r})\right] G_0(\vec{r}t, \vec{r}'t') = \delta(\vec{r}-\vec{r}')\delta(t-t')$

$$\left[i\partial_t - H_0(\vec{r}) - V(\vec{r})\right] G(\vec{r}t, \vec{r}'t') = \delta(\vec{r}-\vec{r}')\delta(t-t')$$

$\downarrow$

$$\left[i\partial_t - H_0(\vec{r})\right] = G_0^{-1}(\vec{r},t)$$

$$\left[i\partial_t - H_0(\vec{r}) - V(\vec{r})\right] = G^{-1}(\vec{r},t)$$

$\downarrow$

$$\psi(\vec{r},t) = \psi^0(\vec{r},t) + \int d^3r' \int dt' \, G_0(\vec{r}t, \vec{r}'t') V(\vec{r}') \psi(\vec{r}',t')$$
$$\psi(\vec{r},t) = \psi^0(\vec{r},t) + \int d^3r' \int dt' \, G(\vec{r}t, \vec{r}'t') V(\vec{r}') \psi^0(\vec{r}',t')$$

$\downarrow$ iterative solution (suppressed integrations)

$$\psi = \psi^0 + G_0 V \psi^0 + G_0 V G_0 V \psi^0 + \dots =$$
$$= \psi^0 + (G_0 + G_0 V G_0 + \dots) V \psi^0 = \psi^0 + G V \psi^0$$

$$\Rightarrow G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \dots =$$
$$= G_0 + G_0 V \underbrace{(G_0 + G_0 V G_0 + \dots)}_{G}$$

$$\Rightarrow \boxed{G = G_0 + G_0 V G}$$

Dyson equation (*)

(*) F. Dyson (1923 - 2020)

G is called "propagator": it propagates wave functions

$$\boxed{\psi(\vec{r},t) = \int d^3r' \int dt' \, G(\vec{r}t, \vec{r}'t') \, \psi(\vec{r}',t')}$$

two solutions for G:

$$G^R(\vec{r}t,\vec{r}'t') = -i\theta(t-t') \langle \vec{r}| e^{-iH(t-t')} |\vec{r}'\rangle$$

retarded

$$G^A(\vec{r}t,\vec{r}'t') = i\theta(t'-t) \langle \vec{r}| e^{-iH(t-t')} |\vec{r}'\rangle$$

advanced

→ amplitude for particle to be in state $(\vec{r},t)$, given it was in state $(\vec{r}',t')$

different basis $|\phi_n\rangle$:

$$G^R(nt,n't') = -i\theta(t-t') \langle \phi_n| e^{-iH(t-t')} |\phi_{n'}\rangle$$

change of basis:

$$G^R(\vec{r}t,\vec{r}'t') = \sum_{nn'} \langle \vec{r}|\phi_n\rangle\, G^R(nt,n't') \langle \phi_{n'}|\vec{r}'\rangle$$

The above considerations and our insights from the Kubo-Nakano formula motivate the definition of the (retarded) many-body Green function

$$\boxed{G^R(\vec{r}\sigma t,\vec{r}'\sigma' t') = -i\theta(t-t') \langle [\psi_\sigma(\vec{r}t), \psi^\dagger_{\sigma'}(\vec{r}'t')]_{B,F} \rangle}$$

$$[A,B]_B = [A,B], \quad [A,B]_F = \{A,B\}$$

$$\psi^\dagger_\sigma(\vec{r}) = \sum_\nu \langle \vec{r}|\psi_\nu\rangle^* a^\dagger_{\nu,\sigma}, \quad \psi_\sigma(\vec{r}) = \sum_\nu \langle \vec{r}|\psi_\nu\rangle a_{\nu,\sigma}$$

for the expectation value $\langle \ldots \rangle$

$$T=0: \langle \ldots \rangle = \langle GS|\ldots|GS\rangle, \quad T\neq 0: \langle \ldots \rangle = \frac{\mathrm{Tr}(\ldots e^{-\beta(H-\mu N)})}{\mathrm{Tr}(e^{-\beta(H-\mu N)})}$$

ground state   grand canonical ensemble

other types of (real-time) Green functions:

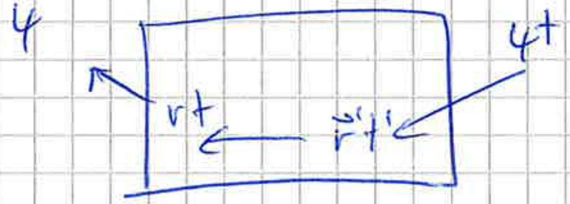
advanced: $G^A(\vec r\sigma t,\vec r'\sigma' t') = i\Theta(t'-t)\langle[\psi_\sigma(\vec r,t),\psi^\dagger_{\sigma'}(\vec r',t')]_{B,F}\rangle$

lesser: $G^<(\vec r\sigma t,\vec r'\sigma' t') = -i(\pm 1)_{B,F}\langle\psi^\dagger_{\sigma'}(\vec r' t')\psi_\sigma(\vec r t)\rangle$

greater: $G^>(\vec r\sigma t,\vec r'\sigma' t') = -i\langle\psi_\sigma(\vec r t)\,\psi^\dagger_{\sigma'}(\vec r' t')\rangle$

causal (time-ordered): $G(\vec r\sigma t,\vec r'\sigma' t') = -i\langle T_t\,\psi_\sigma(\vec r t)\,\psi^\dagger_{\sigma'}(\vec r' t')\rangle$

interpretation of greater GF: inserting a particle at $(\vec r', t')$ taking it out at $(\vec r, t)$



translational invariance

$$G(\vec r,\vec r') \longrightarrow G(\vec r-\vec r')$$

$$G^R(\vec r-\vec r',\sigma t,\sigma' t') = \frac{1}{V}\sum_{\vec k\vec k'} e^{i\vec k\vec r}\, G^R(\vec k\sigma t,\vec k'\sigma' t')\, e^{-i\vec k'\vec r'} =$$

$$= \underbrace{\frac{1}{V}\sum_{\vec k\vec k'} e^{i\vec k(\vec r-\vec r')}\, G^R(\vec k\sigma t,\vec k'\sigma' t')\, e^{i(\vec k-\vec k')\vec r'}}_{\text{cannot depend explicitly on origin, nor } \vec r'}$$

$$\Rightarrow G(\vec k,\vec k') = \delta_{\vec k\vec k'}\, G(\vec k)$$

$$\Rightarrow G^R(\vec r-\vec r',\sigma t,\sigma' t') = \frac{1}{V}\sum_{\vec k} e^{i\vec k(\vec r-\vec r')}\, G(\vec k,\sigma t,\sigma' t')$$

$$G^R(\vec k,\sigma t,\sigma' t') = -i\Theta(t-t')\langle[a_{\vec k\sigma}(t), a^\dagger_{\vec k\sigma'}(t')]_{B,F}\rangle$$

Example: Green function of free electrons (fermions!)

$$H = \sum_{\vec{k}\sigma} \xi_{\vec{k}} c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma}, \quad \xi_{\vec{k}} = \varepsilon_{\vec{k}} - \mu$$

$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ free

$\varepsilon_k = -2t(\cos k_x + \cos k_y)$ tight-binding

...

$$G_0^{>}(k\sigma, t-t') = -i \langle c_{\vec{k}\sigma}(t) c^{\dagger}_{\vec{k}\sigma}(t') \rangle$$

$$c_{\vec{k}\sigma}(t) = e^{iHt} c_{\vec{k}\sigma} e^{-iHt}$$

Heisenberg equation of motion:

- $$\dot{c}_{\vec{k}\sigma}(t) = i[H, c_{\vec{k}\sigma}(t)] = i e^{iHt} [H, c_{\vec{k}\sigma}] e^{-iHt} =$$

$$= i e^{iHt} \sum_{\vec{k}'\sigma'} \xi_{\vec{k}'} [c^{\dagger}_{\vec{k}'\sigma'} c_{\vec{k}'\sigma'}, c_{\vec{k}\sigma}] e^{-iHt}$$

using the identity $[AB, C] = A\{B, C\} - \{A, C\}, B$

$\Downarrow$

$$[c^{\dagger}_{\vec{k}'\sigma'} c_{\vec{k}'\sigma'}, c_{\vec{k}\sigma}] = c^{\dagger}_{\vec{k}'\sigma'} \underbrace{\{c_{\vec{k}'\sigma'}, c_{\vec{k}\sigma}\}}_{\emptyset} - \underbrace{\{c^{\dagger}_{\vec{k}'\sigma'}, c_{\vec{k}\sigma}\}}_{= \{c_{\vec{k}\sigma}, c^{\dagger}_{\vec{k}'\sigma'}\} = \delta_{\vec{k}\vec{k}'}\delta_{\sigma\sigma'}} c_{\vec{k}'\sigma'}$$

$$= -c_{\vec{k}\sigma} \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'}$$

$$\Rightarrow \dot{c}_{\vec{k}\sigma}(t) = i e^{iHt} \sum_{\vec{k}'\sigma'} \xi_{\vec{k}'} (-\delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'}) c_{\vec{k}\sigma} e^{-iHt} =$$

$$= -i\xi_{\vec{k}} e^{iHt} c_{\vec{k}\sigma} e^{-iHt} = -i\xi_{\vec{k}} c_{\vec{k}\sigma}(t)$$

$\Rightarrow$ integration:

$$c_{\vec{k}\sigma}(t) = e^{-i\xi_{\vec{k}} t} c_{\vec{k}\sigma}$$

$$c^{\dagger}_{\vec{k}\sigma}(t) = e^{+i\xi_{\vec{k}} t} c^{\dagger}_{\vec{k}\sigma}$$

$$\Rightarrow G_0^{>}(\vec{k}\sigma, t-t') = \underbrace{-i\langle c_{\vec{k}\sigma} c_{\vec{k}\sigma}^{+}\rangle}_{-i\langle 1 - n_{\vec{k}\sigma}\rangle} e^{-i\xi_{\vec{k}}(t-t')}$$

$\Downarrow$

$n_F(\xi_{\vec{k}})$ ... Fermi function

$\Rightarrow (1-n_F(\xi_{\vec{k}}))$ ... empty state, where e^- is inserted

$e^{-i\xi_{\vec{k}}(t-t')}$ ... plain wave (free!) propagation (no decay!)

$\Rightarrow G_0^{>}$ describes propagation of inserted e^-

Fourier transform (frequency domain)

$$\boxed{G_0^{>}(\vec{k}\sigma, \omega) = -2\pi i\left[1-n_F(\xi_{\vec{k}})\right]\delta(\xi_{\vec{k}}-\omega)}$$

$\Downarrow$

allowed energies ("band structure", "density of states")

Same evaluation possible for:

$$G_0^{<}(\vec{k}\sigma, t-t') = i n_F(\xi_{\vec{k}}) e^{-i\xi_{\vec{k}}(t-t')}$$

$$G_0^{R}(\vec{k}\sigma, t-t') = -i\theta(t-t') e^{-i\xi_{\vec{k}}(t-t')}$$

$$G_0^{A}(\vec{k}\sigma, t-t') = i\theta(t'-t) e^{-i\xi_{\vec{k}}(t-t')}$$