- Time-evolution operator (as an exponential) requires some extra care:

$$\mathcal{U}(t) = e^{-iHt} = e^{-it\sum_{j=1}^{N} h^{(j)}} = u(t) \otimes \cdots\cdots \otimes u(t)$$ with N identical factors $u(t) = e^{-iht}$.

$\rightsquigarrow$ $\mathcal{U}(t)$ <u>not</u> of conventional one-body form $\sum_i \mathcal{O}^{(i)}$, even if H itself is!

– Application to time evolved expectation values of one-body operators:

$$\langle \Psi_0 | \mathcal{U}^+(t)\, \mathcal{O}\, \mathcal{U}(t) | \Psi_0 \rangle = \langle \Psi_0 | \sum_{i=1}^{N} \underbrace{(\mathcal{U}^+(t)\, \mathcal{O}\, \mathcal{U}(t))^{(i)}}_{\equiv\, \mathcal{O}^{(i)}(t)} | \Psi_0 \rangle =$$

$$= \sum_i \langle \alpha_i | \mathcal{O}(t) | \alpha_i \rangle .$$

$\rightsquigarrow$ $\mathcal{O}(t)$ still behaves like an ordinary one-body operator.

– Application to overlaps between time-evolved and initial state (auto-correlations)

$$\langle \Psi_0 | \Psi(t) \rangle = \langle \Psi_0 | U(t) | \Psi_0 \rangle \overset{\text{Fermions}}{=} \frac{1}{N!} \sum_{P,P'} (-)^{|P|+|P'|} \times$$

$$\times \langle \alpha_1, \dots, \alpha_N | P^{\dagger} U(t) P' | \alpha_1, \dots, \alpha_N \rangle \underset{[P,U]=0}{=}$$

$$= \frac{1}{N!} \sum_{P,P'} (1)^{|P|+|P'|} \langle \alpha_1, \dots, \alpha_N | U(t) \underbrace{P^{\dagger} P'}_{\tilde{P}} | \alpha_1, \dots, \alpha_N \rangle =$$

$$= \sum_{\tilde{P}} (-1)^{|\tilde{P}|} \langle \alpha_1, \dots \alpha_N | U(t) \tilde{P} | \alpha_1, \dots, \alpha_N \rangle =$$

$$= \sum_{\tilde{P}} (-1)^{|\tilde{P}|} \prod_{i=1}^{N} \langle \alpha_i | U(t) | \alpha_{\tilde{P}(i)} \rangle \underset{\text{Def. determinant}}{=} \det\left(\left(\langle \alpha_i | U(t) | \alpha_j \rangle \right)_{ij} \right).$$

$\rightsquigarrow$ Analogous calculation for bosons $\langle \Psi_0 | \Psi(t) \rangle = \underset{\substack{\uparrow \\ \text{permanent}}}{\mathrm{per}} \left(\left(\langle \alpha_i | U(t) | \alpha_j \rangle \right)_{ij} \right)$

! Permanent cannot be calculated efficiently for general matrix !

$\rightsquigarrow$ Work around for Gaussian states, i.e. thermal states of a quadratic Hamiltonian.

With $|\Psi_0\rangle = \lim\limits_{\beta \to \infty} \frac{e^{-\beta \tilde{H}}}{\mathrm{Tr}(e^{-\beta \tilde{H}})}$ for some one-body Hamiltonian $\tilde{H}$,

consider $\langle \Psi_0 | \Psi(t) \rangle = \lim\limits_{\beta \to \infty} \mathrm{Tr}_{\mathcal{H}_F^+} \left(\frac{e^{-\beta \tilde{H}}}{\mathrm{Tr}_{\mathcal{H}_F^+}(e^{-\beta \tilde{H}})} e^{-iHt} \right)$ and use

$$\mathrm{Tr}_{\mathcal{H}_F^+} \left(e^{O_1} e^{O_2} \right) = \det \left(1 - e^{O_1} e^{O_2} \right)^{-1} \text{ for } O_1 = -\beta \tilde{H} \text{ and } O_2 = -iHt.$$

- General (particle number conserving) n-body operators:

$$O = \sum_{\substack{\alpha_1, \dots, \alpha_n \\ \beta_1, \dots, \beta_n}} O^{\alpha_1 \dots \alpha_n}_{\beta_1 \dots \beta_n} a^\dagger_{\alpha_1} \dots a^\dagger_{\alpha_n} a_{\beta_n} \dots a_{\beta_1}$$

$$\langle \Psi | O | \Psi \rangle \underset{\substack{\uparrow \\ |\Psi\rangle \text{ uncorrelated}}}{=} \sum_{\substack{\alpha_1 \dots \alpha_n \\ \beta_1 \dots \beta_n}} \underbrace{\langle \Psi | a^\dagger_{\alpha_1} \dots a^\dagger_{\alpha_n} a_{\beta_n} \dots a_{\beta_1} | \Psi \rangle}_{\equiv (\mathrm{I})} O^{\alpha_1 \dots \alpha_n}_{\beta_1 \dots \beta_n}$$

$$(\mathrm{I}) \underset{\substack{\uparrow \\ \text{Wick's theorem}}}{=} \sum_{\substack{\text{all pairings} \\ P}} (\pm 1)^{|P|} \left(\langle \Psi | a^{\dagger}_{\alpha_1} a_{\beta_{P(1)}} | \Psi \rangle \cdots \langle \Psi | a^{\dagger}_{\alpha_n} a_{\beta_{P(n)}} | \Psi \rangle \right).$$

Recap: Green's functions in free systems

- Basic idea: Green's functions are correlation functions that describe excitations and their propagation in QMB systems.
  ↳ Many physical properties such as response functions to probe fields are determined by Green's functions.
  ↳ Green's functions (GFs) are the crucial quantities for perturbation theory in QMB systems.

Mathematical basics on Green's functions:

- Consider <u>linear</u> inhomogeneous differential equation

$$D_x u(x) = h(x) \text{ with homogeneous solution } D_x u_0(x) = 0$$

- GF defined by $D_x G(x,x') = \delta(x-x')$
- General solution then reads as $u(x) = u_0(x) + \int dx'\, G(x,x')\, h(x')$
- Check: $D_x u(x) = \underbrace{D_x u_0(x)}_{=0} + \int dx' \underbrace{D_x G(x,x')}_{\delta(x-x')} h(x') = h(x)$ ✓

- Paradigmatic example in physics: Retarded GF of a (free) fermionic system:

$$G^r(x,t;x',t') = -i\theta(t-t') \langle \{ \Psi(\vec{x},t), \Psi^\dagger(\vec{x}',t') \} \rangle$$

Heisenberg picture

- For a translation-invariant system with time-independent Hamiltonian, we get $G^r(x,t;x',t') \equiv G^r(x-x', t-t')$ and on Fourier transform

$$G^r(x-x', t-t') \to G^r(k,\omega).$$

– Consider free system with $H_0 = \sum_k \varepsilon_k a_k^+ a_k$.

$$\rightsquigarrow \quad G_0^r(k, t-t') = -i\,\theta(t-t')\, e^{-i\varepsilon_k(t-t')} \langle \underbrace{\{a_k, a_k^+\}}_{=1} \rangle = -i\,\theta(t-t')\, e^{-i\varepsilon_k(t-t')}.$$

free

With $\theta(t-t') \overset{\substack{\text{residue}\\ \text{theorem}}}{=} \lim_{\eta \to 0^+} \frac{-1}{2\pi i} \int_{-\infty}^{\infty} d\omega' \, e^{-i\omega'(t-t')} \frac{1}{\omega' + i\eta}$, we obtain

$$G_0^r(k, \omega) = \int_{-\infty}^{+\infty} d(t-t')\, e^{i\omega(t-t')} G_0^r(k, t-t') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d(t-t') \int_{-\infty}^{\infty} d\omega' \, e^{i(\omega - \varepsilon_k - \omega')(t-t')} \frac{1}{\omega' + i0^+}$$

$$= \int_{-\infty}^{\infty} d\omega' \, \delta(\omega - \omega' - \varepsilon_k) \frac{1}{\omega' + i0^+} = \frac{1}{\omega + i0^+ - \varepsilon_k} = \langle k | (\omega + i0^+ - H_0)^{-1} | k \rangle.$$

$\rightsquigarrow$ G_0^r corresponds to the (shifted) inverse of the free Hamiltonian.

– Equation of motion: $i\partial_t G_0^r(k, t-t') = \delta(t-t') + \varepsilon_k \underbrace{\left(-i\theta(t-t')\, e^{-i\varepsilon_k(t-t')}\right)}_{= G_0^r(k, t-t')}$

$$\Leftrightarrow \quad (i\partial_t - \varepsilon_k)\, G_0^r(k, t-t') = \delta(t-t')$$

$\rightsquigarrow$ G_0^r is a Green's function of the free Schrödinger equation in the conventional mathematical sense.