Quantum kinetic equations
Lecture #1

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December 3, 2008

Outline

Quick review on the quantum harmonic oscillator

Hamiltonian of a single particle (of mass m) moving in a parabolic confinement of frequency ω (harmonic oscillator)

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2\hat{x}^2 \,, \qquad \hat{p} = -i\hbar\nabla$$

Canonical commutation relation:

$$[\hat{x}, \hat{p}]_- = i\hbar \,, \qquad [A, B]_\pm = \hat{A}\hat{B} \pm \hat{B}\hat{A}$$

Alternative formulation:

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

with creation and annihilation operators

$$\hat{a} = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}\hat{x} + i\frac{\hat{p}}{\sqrt{m\omega\hbar}}\right] \,, \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left[\sqrt{\frac{m\omega}{\hbar}}\hat{x} - i\frac{\hat{p}}{\sqrt{m\omega\hbar}}\right]$$

Quick review on the quantum harmonic oscillator

Action onto an arbitrary state $|n\rangle$, $n = 0, 1, \ldots$

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle \;, \qquad \hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle$$

Properties:

$$[\hat{a}, \hat{a}^\dagger]_- = 1 \;, \qquad [\hat{a}, \hat{a}]_- = 0 \;, \qquad [\hat{a}^\dagger, \hat{a}^\dagger]_- = 0$$

Occupation number operator $\hat{n} = \hat{a}^\dagger \hat{a}$ obeys $\hat{n}\,|n\rangle = n\,|n\rangle$

Direct way for solution:

- Ground state: $\hat{a}\,|0\rangle = 0$ ($|0\rangle$: vacuum state) $\Rightarrow$ differential equation for $\psi_0(x) = \langle x|0\rangle$ with solution $\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$ and energy eigenvalue $E_0 = \hbar\omega/2$
- Excited states: $\psi_n(x) = \frac{1}{\sqrt{n!}} \langle x|\,(a^\dagger)^n\,|0\rangle$, $E_n = \hbar\omega(n + \frac{1}{2})$

Idea of second quantization

Single harmonic oscillator $\Longrightarrow$ Generalizations: **Coupled** harmonic oscillators

- Extend concept of single-particle creation (annihilation) operators to **interacting** many-body systems
- Account for the correct fermionic (bosonic) symmetry—include Fermi-Dirac (Bose-Einstein) statistics
- Reformulation where symmetry relations of bosonic <u>and</u> fermionic wavefunctions are naturally (automatically) included
- Allow for states with variable particle number $\rightarrow$ Fock space!

Idea of second quantization

Fock space:

- Denote by $\mathcal{H}_N$ the Hilbert space for N particles.
- The Fock space is the direct sum

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \ldots \oplus \mathcal{H}_N \oplus \ldots$$

- An arbitrary state $|\psi\rangle$ in Fock space is the sum over all subspaces $\mathcal{H}_N$

$$|\psi\rangle = |\psi^{(0)}\rangle + |\psi^{(1)}\rangle + \ldots + |\psi^{(N)}\rangle + \ldots$$

- The subspace $\mathcal{H}_0$ is one-dimensional spanned by vector $|0\rangle$ (vacuum)
- Inner product $\langle\chi|\psi\rangle = \sum_{j=0}^{\infty}\langle\chi^{(j)}|\psi^{(j)}\rangle$ vanishes, if $|\chi\rangle$ and $|\psi\rangle$ belong to different subspaces (orthogonality)
- Full support for (anti)symmetry of the many-body state
- Particle number is not fixed a-priori. Statistical physics picture: CE (canonical ensemble) $\rightarrow$ GCE (grand canonical ensemble)

Idea of second quantization

Creation and annihilation operators:

- **Example**: Consider $|\psi^{(N)}\rangle \in \mathcal{H}_N$ being constructed from 1-particle states ψ_k with $k = 1, 2, \ldots, N$, i.e. $|\psi^{(N)}\rangle = |\psi_1, \ldots, \psi_N\rangle$
- Let $|\phi\rangle \in \mathcal{H}_1$ be an arbitrary one-particle state (no particular representation)
  Creation operator:

$$\hat{a}^\dagger(\phi)\,|\psi^{(N)}\rangle \;=\; \hat{a}^\dagger(\phi)\,|\psi_1, \ldots, \psi_N\rangle = |\phi, \psi^{(N)}\rangle$$

  Destruction/annihilation operator:
  (upper sign = bosons, lower sign = fermions)

$$\langle\chi^{(N-1)}|\,\hat{a}(\phi)\,|\psi^{(N)}\rangle \;=\; \langle\psi^{(N)}|\,\hat{a}^\dagger(\phi)\,|\chi^{(N-1)}\rangle^*$$

$$\hat{a}(\phi)\,|\psi^{(N)}\rangle \;=\; \sum_{k=1}^{N}(\pm)^{k-1}\langle\phi|\psi_k\rangle\,|\psi_1, \ldots, \psi_{k-1}, \psi_{k+1}, \ldots, \psi_N\rangle$$

- Fermi or Bose statistics enter via (anti-)commutation relations

$$\left[\hat{a}^\dagger(\phi_1), \hat{a}^\dagger(\phi_2)\right]_\mp = 0\,, \quad [\hat{a}(\phi_1), \hat{a}(\phi_2)]_\mp = 0\,, \quad \left[\hat{a}(\phi_1), \hat{a}^\dagger(\phi_2)\right]_\mp = \langle\phi_1|\phi_2\rangle$$

Idea of second quantization

- Changing between different one-particle representations:

Let $\{|\chi_i\rangle\}$ and $\{|\phi_i\rangle\}$ be two distinct complete sets of one-particle states corresponding to an N-particle system.

The annihilation (creation) operators $a^{(\dagger)}(\chi_i)$ in the representation $|\chi_i\rangle$ are then obtained from $a^{(\dagger)}(\phi_\alpha)$ by the following transformation:

$$\hat{a}^\dagger(\chi_i) = \sum_\alpha \langle\phi_\alpha|\chi_i\rangle\, \hat{a}^\dagger(\phi_\alpha)\;, \qquad \hat{a}(\chi_i) = \sum_\alpha \langle\chi_i|\phi_\alpha\rangle\, \hat{a}(\phi_\alpha)\;,$$

with coefficients $\langle\phi_\alpha|\chi_i\rangle$ and $\langle\chi_i|\phi_\alpha\rangle$, respectively.

Second quantized Hamiltonian

Consider N identical non-relativistic particles represented by a coordinate wave function $\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$, with $\mathbf{r}_i$ labeling coordinate and spin.

Hamiltonian (1^{st} quantization):

$$\hat{H}(t) = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla^2_{\mathbf{r}_i} + \sum_{i=1}^{N} V(\mathbf{r}_i, t) + \sum_{i<j} W(\mathbf{r}_i - \mathbf{r}_j)$$

Hamiltonian (2^{nd} quantization):

- In position space representation $\hat{a}^{(\dagger)}(\phi) \rightarrow \hat{\Psi}^{(\dagger)}(\mathbf{r})$
- $\hat{\Psi}^{\dagger}(\mathbf{r})$, $\hat{\Psi}(\mathbf{r})$ in this represantation are called "field operators"

(Anti-)commutation relations (bosons/fermions): more

$$[\hat{\Psi}^{(\dagger)}(\mathbf{r}_1), \hat{\Psi}^{(\dagger)}(\mathbf{r}_2)]_{\mp} = 0 \,, \qquad [\hat{\Psi}(\mathbf{r}_1), \hat{\Psi}^{\dagger}(\mathbf{r}_2)]_{\mp} = \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

Second quantized Hamiltonian

Hamiltonian (2^{nd} quantization)—continued: more

$$\hat{H}(t) = \int \mathrm{d}^3 r\, \hat{\Psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t) \right] \hat{\Psi}(\mathbf{r}) + \frac{1}{2} \iint \mathrm{d}^3 r\, \mathrm{d}^3 \bar{r}\; \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\bar{\mathbf{r}}) w(\mathbf{r}-\bar{\mathbf{r}}) \hat{\Psi}(\bar{\mathbf{r}}) \hat{\Psi}(\mathbf{r}) \quad (1)$$

- general result for fermions *and* bosons
- $\hat{H}(t)$ commutes with the total number operator $\hat{N} = \int \mathrm{d}^3 r\; \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r})$, since $\hat{H}(t)$ conserves total number of particles
- Fock space picture related to GCE suggests fixing the particle number via chemical potential μ (Lagrange multiplier) in order to weight contributions from different parts of the Fock space $\mathcal{H}$
- Require the average particle number $\langle \hat{N} \rangle$ to be fixed. Define:

$$\tilde{H}(t) = \hat{H}(t) - \mu \hat{N}$$

Heisenberg picture and ensemble averages

Goal: development of a time-dependent quantum many-body theory

Heisenberg picture:

- Operators become explicitly time-dependent, $|\psi^{(N)}\rangle = \text{const}$
- In particular, $\hat{\Psi}^{(\dagger)}(\mathbf{r}) \to \hat{\Psi}^{(\dagger)}_H(\mathbf{r}, t) = \hat{U}^\dagger(t, t_0)\, \hat{\Psi}^{(\dagger)}(\mathbf{r})\, \hat{U}(t, t_0)$ with time-evolution operator

$$\hat{U}(t, t_0) = \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}\bar{t}\, \tilde{H}(\bar{t})\right)\,, \qquad \hat{U}^\dagger(t, t_0) = \hat{U}(t_0, t)$$

- Heisenberg equation $\frac{\partial}{\partial t}\hat{\Psi}^{(\dagger)}_H(\mathbf{r}, t) = -i\left[\tilde{H}, \hat{\Psi}^{(\dagger)}_H(\mathbf{r}, t)\right]_-$

Ensemble averages of $\hat{\Psi}^{(\dagger)}_H(\mathbf{r}, t)$:

- Single-field operator randomly fluctuating, expectation values $\langle \Psi^{(\dagger)}_H(\mathbf{r}, t)\rangle$ ($\langle \ldots \rangle = \mathrm{Tr}\{\hat{\rho}\ldots\}$) often vanish
- Need **two-operator averages**

  (compare with harmonic oscillator: two-operator product $\langle \hat{n}\rangle = \langle \hat{a}^\dagger \hat{a}\rangle$ yields average occupation number)

Nonequilibrium Green's functions $G^{\gtrless}(1,\bar{1})$

Nonequilibrium Green's functions (NEGF):

- $\hat{\Psi}^\dagger_H(\mathbf{r},t)$, $\hat{\Psi}_H(\mathbf{r},t)$ are non-commuting $\Rightarrow$ in nonequilibrium exist two possible independent combinations

Correlation functions $G^{\gtrless}$

$$G^<(1,\bar{1}) = \pm\frac{1}{i\hbar}\left\langle \hat{\Psi}^\dagger_H(\bar{1})\hat{\Psi}_H(1)\right\rangle$$
$$G^>(1,\bar{1}) = \frac{1}{i\hbar}\left\langle \hat{\Psi}_H(1)\hat{\Psi}^\dagger_H(\bar{1})\right\rangle$$

coordinate representation, $1=\mathbf{r}_1,t_1$, $\bar{1}=\mathbf{r}_{\bar{1}},t_{\bar{1}}$, and $\langle\ldots\rangle = \mathrm{Tr}\{\hat{\rho}\ldots\}$

- Connection with reduced density matrix (time-diagonal element)

$$\rho(\mathbf{r}_1,\mathbf{r}_{\bar{1}};T) = \pm i\hbar G^<(1,\bar{1})|_{t_1=t_{\bar{1}}=T}$$

- Relative and center-of-mass variables $T=(t_1+t_{\bar{1}})/2$, $t=t_1-t_{\bar{1}}$, $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_{\bar{1}})/2$, and $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_{\bar{1}}$ often useful

Nonequilibrium Green's functions $G(1,\bar{1})$

Recall: Vacuum field theory uses time-ordered products

$\Rightarrow$ Perturbation theory, Wick theorem, Feynman diagrams

Thus define

Time-ordered 1-particle Green's function:

$$
\begin{aligned}
G(1,\bar{1}) &= -i \left\langle T_{\mathscr{C}}\, \hat{\Psi}_H(1)\, \hat{\Psi}^\dagger_H(\bar{1}) \right\rangle \\
&= \theta(t_1, t_{\bar{1}})\, G^>(1,\bar{1}) - \theta(t_{\bar{1}}, t_1)\, G^<(1,\bar{1})
\end{aligned}
$$

- From now on take $\hbar \equiv 1$
- Formally, the operator $T_{\mathscr{C}}$ ensures time-ordering

Time-ordered 2-particle Green's function:

$$
G_{12}(1,2;\bar{1},\bar{2}) = (-i)^2 \left\langle T_{\mathscr{C}}\, \hat{\Psi}_H(1)\, \hat{\Psi}_H(2)\, \hat{\Psi}^\dagger_H(\bar{2})\, \hat{\Psi}^\dagger_H(\bar{1}) \right\rangle
$$

Information contained in $G(1,\bar{1})$

One-particle density[1]

$$\langle\hat{n}\rangle(\mathbf{r}_1,t_1) = -i\,G(1,1^+) = \pm i\,G^<(\mathbf{r}_1 t_1,\mathbf{r}_1 t_1)$$

Particle number

$$\langle\hat{N}\rangle(t_1) = -i\int \mathrm{d}^3 r_1\,G(1,1^+)$$

Charge current density (in absence of any vector potential $A(\mathbf{r},t)$)

$$\langle\mathbf{j}\rangle(1) = \pm i\left\{\frac{\nabla_{\mathbf{r}_1}-\nabla_{\mathbf{r}_2}}{2im}G^<(1,\mathbf{r}_2 t_1)\right\}_{\mathbf{r}_1=\mathbf{r}_2}$$

Total energy (2-particle quantity)

$$\langle\hat{E}\rangle(t_1) = \pm i\int \mathrm{d}^3 r_1\left\{\frac{1}{2}(i\frac{\partial}{\partial t_1}+H^0(1)-2\mu)G(1,\bar{1})\right\}_{1=\bar{1}}$$

with one-particle (energy) operator $H^0(1) = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_1} + V(\mathbf{r}_1,t)$

[1] notation 1^+ indicates $t_1 \to t_1+\epsilon,\ \epsilon>0$

Information contained in $G(1, \bar{1})$

Wigner function:

$$f(\mathbf{p}, \mathbf{R}, T) = \pm \frac{i}{2\pi} \int \mathrm{d}\omega \, G(\mathbf{p}, \omega; \mathbf{R}, T)$$

- $f(\mathbf{p}, \mathbf{R}, T)$ is central quantity in the Wigner representation of a reduced density operator theory ▸ $G(\mathbf{p}, \omega; \mathbf{R}, T)$

Spectral function: ▸ more

$$A(1, \bar{1}) = i\{G^{>}(1, \bar{1}) - G^{<}(1, \bar{1})\}$$

- Gives DOS by Fourier transform with respect to relative time t (in general space-time dependent and momentum resolved)
- Integration over remaining degrees of freedom in $G(\mathbf{p}, \omega; \mathbf{R}, T) \to A(\omega)$ (pure DOS)

Time-dependent observables

Evolution of an observable $\langle \hat{O} \rangle$ in the GCE:

Assume $\tilde{H}(t \leq t_0) = \tilde{H}_0$ is time-independent for $t \leq t_0$

$$\langle \hat{O} \rangle(t) = \mathrm{Tr}\left\{ \hat{\rho}\, \hat{O}_H(t) \right\} , \qquad \hat{\rho} = \frac{e^{-\beta \tilde{H}_0}}{\mathrm{Tr}\left\{ e^{-\beta \tilde{H}_0} \right\}} , \qquad \hat{O}_H(t) = \hat{U}(t_0, t) \hat{O} \hat{U}(t, t_0)$$

$$\text{time-evolution operator } \hat{U}(t, t_0) = \exp\left(-i \int_{t_0}^{t} \mathrm{d}\bar{t}\ \tilde{H}(\bar{t}) \right)$$

Consider: $\hat{U}(t_0 - i\beta, t_0)$

$$\hat{U}(t_0 - i\beta, t_0) = \exp\left(-i \left[\tilde{H}_0\, \bar{t} \right]_{t_0}^{t_0 - i\beta} \right) = \exp\left(-\beta \tilde{H}_0 \right)$$

density operator

Result:

$$\langle \hat{O} \rangle(t) = \frac{\mathrm{Tr}\left\{ \hat{U}(t_0 - i\beta, t_0)\, \hat{U}(t_0, t)\, \hat{O}\, \hat{U}(t, t_0) \right\}}{\mathrm{Tr}\left\{ \hat{U}(t_0 - i\beta, t_0) \right\}}$$

- Interpretation: time-evolution $t_0 \to t$, action of $\hat{O}$, $t \to t_0$, $t_0 \to t_0 - i\beta$

▸ more

Complex-time Schwinger/Keldysh contour $\mathscr{C}'$

- Introduce deformed time-contour: Schwinger/Keldysh contour $\mathscr{C}'$

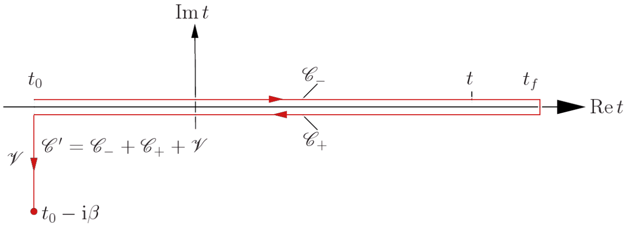


Figure: Full Keldysh contour $\mathscr{C}' = \{t \in \mathbb{C} | \mathfrak{Im}\, t \in [-\beta, 0], \mathfrak{Re}\, t \in [t_0, \infty]\}$

- **Need**: Statistical average of the time-ordered field-operator product
- Consequently, $\mathscr{V}$ also enters in the 1-particle Green's function $G(1, \bar{1}) = -i\langle T_{\mathscr{C}'}\, \hat{\Psi}_h(1)\, \hat{\Psi}^\dagger_H(\bar{1})\rangle$ giving rise to subordinated Green's functions which exist on different contour branches $\mathscr{C}$ and $\mathscr{V}$, or on $\mathscr{V}$ only.

$\Longrightarrow$ two mixed functions ($G^{\lceil}$, $G^{\rceil}$) and the Matsubara Green's function G^M

more

Equations of motions for $G(1, \bar{1})$

1. Starting point: Heisenberg equation for $\hat{\Psi}_H(\mathbf{r}, t)$ and $\hat{\Psi}^\dagger_H(\mathbf{r}, t)$

$$\frac{\partial}{\partial t}\hat{\Psi}^{(\dagger)}_H(\mathbf{r}, t) = -i\left[\tilde{H}, \hat{\Psi}^{(\dagger)}_H(\mathbf{r}, t)\right]_-$$

It follows ($1 = \mathbf{r}_1, t_1;\ \bar{1} = \mathbf{r}_{\bar{1}}, t_{\bar{1}}$)

$$\left(i\frac{\partial}{\partial t_1} + \frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_1} - V(1) + \mu\hat{N}\right)\hat{\Psi}_H(1) = \int_{\mathscr{C}'} \mathrm{d}\bar{1}\, W(1-\bar{1})\,\hat{\Psi}^\dagger_H(\bar{1})\,\hat{\Psi}_H(\bar{1})\,\hat{\Psi}_H(1)$$

- Definition: Use short notation $\int_{\mathscr{C}'}\mathrm{d}\bar{1} = \int_{\mathscr{C}'}\mathrm{d}t_{\bar{1}} \int \mathrm{d}^3 r_{\bar{1}}$
- Instantaneous pair interaction $W(1-\bar{1}) = w(\mathbf{r}_1 - \mathbf{r}_{\bar{1}})\delta_{\mathscr{C}'}(t_1 - t_{\bar{1}})$
- Closed equation for $\hat{\Psi}_H(1)$, adjoint equation for $\hat{\Psi}^\dagger_H(1)$
- Goal: nonzero combination of field operators ($\rightarrow$ NEGF)

Equations of motions for $G(1,\bar{1})$

2. Proceed: Multiplication by $(-i)\Psi_H^{(\dagger)}(\mathbf{r}_{\bar{1}},t_{\bar{1}})$, time-ordering $T_{\mathscr{C}'}$, and ensemble averaging $\langle\ldots\rangle$

- l.h.s. using $H^1(1) = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_1} + V(1) - \mu\hat{N}$

$$\begin{aligned}
&(-i)\left\langle T_{\mathscr{C}'}\left[\left(i\frac{\partial}{\partial t_1} - H^1(1)\right)\hat{\Psi}_H(1)\,\hat{\Psi}_H^\dagger(\bar{1})\right]\right\rangle \\
=\;& i(-i)\left\langle T_{\mathscr{C}'}\left[\frac{\partial}{\partial t_1}\hat{\Psi}_H(1)\,\hat{\Psi}_H^\dagger(\bar{1})\right]\right\rangle - H^1(1)\,(-i)\left\langle T_{\mathscr{C}'}\,\hat{\Psi}_H(1)\,\hat{\Psi}_H^\dagger(\bar{1})\right\rangle \\
=\;& \left(i\frac{\partial}{\partial t_1} - H^1(1)\right)G(1,\bar{1}) - \delta_{\mathscr{C}}(1-\bar{1})
\end{aligned}$$

- r.h.s. $\quad 2^+$ indicates $t_2 \to t_2 + \epsilon$, $\epsilon > 0$

$$\begin{aligned}
&(-i)\int_{\mathscr{C}'} \mathrm{d}2\, W(1-2)\,\left\langle T_{\mathscr{C}'}\hat{\Psi}_H^\dagger(2^+)\,\hat{\Psi}_H(2)\,\hat{\Psi}_H(1)\,\hat{\Psi}_H^\dagger(\bar{1})\right\rangle \\
=\;& \pm i(-i)^2\int_{\mathscr{C}'} \mathrm{d}2\, W(1-2)\,\left\langle T_{\mathscr{C}'}\hat{\Psi}_H(1)\,\hat{\Psi}_H(2)\,\hat{\Psi}_H^\dagger(2^+)\,\hat{\Psi}_H^\dagger(\bar{1})\right\rangle \\
=\;& \pm i\int_{\mathscr{C}'} \mathrm{d}2\, W(1-2)\,G_{12}(1,2;\bar{1},2^+)
\end{aligned}$$

Kadanoff-Baym/Keldysh equations

3. Additionally: Adjoint equation with times t_1 and $t_{\bar{1}}$ interchanged

Kadanoff-Baym/Keldysh equations (KBE)—Summary

$$\left(i\frac{\partial}{\partial t_1} - H^1(1)\right) G(1,\bar{1}) = \delta_{\mathscr{C}'}(1-\bar{1}) \pm i\int_{\mathscr{C}'} d2\, W(1-2)\, G_{12}(1,2;\bar{1},2^+)$$

$$\left(-i\frac{\partial}{\partial t_{\bar{1}}} - H^1(\bar{1})\right) G(1,\bar{1}) = \delta_{\mathscr{C}'}(1-\bar{1}) \pm i\int_{\mathscr{C}'} d2\, W(\bar{1}-2)\, G_{12}(1,2;\bar{1},2^+)$$

- Coupled pair of first order integro-differential equations in the time arguments $t_1, t_{\bar{1}} \in \mathscr{C}'$
- $H^1(1) = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_1} + V(1) - \mu\hat{N}$ denotes the single-particle Hamiltonian
- KBE not closed but coupled to higher orders via the 2-particle Green's function $G_{12}(1,2;\bar{1},\bar{2}) \Longrightarrow$ *Martin-Schwinger hierarchy* (generalization of BBGKY hierarchy): The n-particle Green's function generally requires information from the $(n\pm 1)$-particle Green's function
- KBE must be supplied with initial boundary (or initial) conditions

KBE—boundary or initial conditions

Apply either

- *Kubo-Martin-Schwinger* (KMS) boundary conditions[2]:

  (known from equilibrium theory)

$$
\begin{aligned}
G(\mathbf{r}_1 t_0, \bar{1}) &= \pm G(\mathbf{r}_1 t_0 - i\beta, \bar{1}) \\
G(1, \mathbf{r}_{\bar{1}} t_0) &= \pm G(1, \mathbf{r}_{\bar{1}} t_0 - i\beta)
\end{aligned}
$$

  - (Anti-)periodicity in the inverse temperature β for bosons (fermions)
  - compute equilibrium Green's function prior to time-propagation—systematic and consistent approach

or

- Initial conditions (Kadanoff/Baym):

  from given spectral and Wigner function, A and f construct:

$$
\begin{aligned}
iG^{>}(\mathbf{p}, \omega; \mathbf{R}, t_0) &= A(\mathbf{p}, \omega; \mathbf{R}, t_0)\,[1 \pm f(\mathbf{p}, \omega; \mathbf{R}, t_0)] \\
\pm iG^{<}(\mathbf{p}, \omega; \mathbf{R}, t_0) &= A(\mathbf{p}, \omega; \mathbf{R}, t_0)\, f(\mathbf{p}, \omega; \mathbf{R}, t_0)
\end{aligned}
$$

[2] obtained from the cyclic property of the trace

Conclusion

- 1-particle Green's function: function of two space-time variables. Equation of motion: KBE
- From $G(1,\bar{1})$ one can calculate time-dependent expectation values such as currents densities, total energy etc.

Why nonequilibrium Green's functions?

- Without external field: NEGF naturally reduces to equilibrium (Matsubara) Green's functions
- Applicable to arbitrary nonequilibrium processes
- Can handle strong external fields nonperturbatively

$\longrightarrow$ next lecture:

- Conserving approximations (hierarchy decoupling), memory effects/kernels
- Inclusion of particle-particle interactions via infinite summations (self-energy)

Fin

Thanks for your attention!

Next lecture: (i) Hierarchy decoupling, self-energies and Feynman diagrams
(ii) Single-time kinetic equations

Creation and annihilation operators ◂ back

Action of $\hat{\Psi}^{(\dagger)}(\mathbf{r})$ on a N-particle state $\psi^N(\mathbf{r}_1, \ldots, \mathbf{r}_N)$:

- Particle destruction/annihilation

$$\hat{\Psi}(\mathbf{r})\,\psi^{(N)}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \quad = \quad \sqrt{N}\,\psi^{(N)}(\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}, \mathbf{r})$$

- Particle creation

$$\hat{\Psi}^{\dagger}(\mathbf{r})\,\psi^{(N)}(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

$$= \quad \frac{(\pm 1)^N}{\sqrt{N+1}} \sum_{j=1}^{N+1} (\pm 1)^{j+1} \delta(\mathbf{r} - \mathbf{r}_j)\,\psi^{(N)}(\mathbf{r}_1, \ldots, \mathbf{r}_{j-1}, \mathbf{r}_{j+1}, \ldots, \mathbf{r}_{N+1})$$

Second quantized Hamiltonian ◂ back

Example: Kinetic energy operator $\hat{T} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N} \nabla^2_{\mathbf{r}_i}$ in 2^{nd} quantization

$$\hat{T} = -\frac{\hbar^2}{2m}\int \mathrm{d}^3 r\; \hat{\Psi}^\dagger(\mathbf{r})\, \nabla^2_{\mathbf{r}}\, \hat{\Psi}(\mathbf{r})$$

Proof:

$$\begin{aligned}
\hat{T}\psi^{(N)}(\mathbf{r}_1,\ldots,\mathbf{r}_N) &= -\frac{\hbar^2}{2m}\int \mathrm{d}^3 r\; \nabla^2_{\bar{\mathbf{r}}}\, \hat{\Psi}^\dagger(\mathbf{r})\, \hat{\Psi}(\bar{\mathbf{r}})\, \psi^{(N)}(\mathbf{r}_1,\ldots,\mathbf{r}_N)\Big|_{\bar{\mathbf{r}}=\mathbf{r}} \\
&= -\frac{\hbar^2}{2m}\int \mathrm{d}^3 r\; \nabla^2_{\bar{\mathbf{r}}}\, \hat{\Psi}^\dagger(\mathbf{r})\, \sqrt{N}\, \psi^{(N)}(\mathbf{r}_1,\ldots,\mathbf{r}_{N-1},\bar{\mathbf{r}})\Big|_{\bar{\mathbf{r}}=\mathbf{r}} \\
&= -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\int \mathrm{d}^3 r\; \nabla^2_{\bar{\mathbf{r}}}\, \delta(\mathbf{r}-\mathbf{r}_i)\, \psi^{(N)}(\mathbf{r}_1,\ldots,\mathbf{r}_{i-1},\bar{\mathbf{r}},\mathbf{r}_{i+1},\ldots,\mathbf{r}_N)\Big|_{\bar{\mathbf{r}}=\mathbf{r}} \\
&= -\frac{\hbar^2}{2m}\sum_{i=1}^{N} \nabla^2_{\mathbf{r}}\, \psi^{(N)}(\mathbf{r}_1,\ldots,\mathbf{r}_{i-1},\mathbf{r},\mathbf{r}_{i+1},\ldots,\mathbf{r}_N) \\
&= \left(-\frac{\hbar^2}{2m}\sum_{i=1}^{N} \nabla^2_{\mathbf{r}_i}\right) \psi^{(N)}(\mathbf{r}_1,\ldots,\mathbf{r}_N)
\end{aligned}$$

$G^{\gtrless}$ in relative and center of mass coordinates

back

We recall that

$$G^{<}(\mathbf{p}\omega, \mathbf{R}T) = \int d^3r\, dt\; e^{-i\mathbf{p}\mathbf{r}+i\omega t}\, [\pm i G^{<}(\mathbf{r}t, \mathbf{R}T)]$$

$$G^{>}(\mathbf{p}\omega, \mathbf{R}T) = \int d^3r\, dt\; e^{-i\mathbf{p}\mathbf{r}+i\omega t}\; i\, G^{>}(\mathbf{r}t, \mathbf{R}T)$$

$$\mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_{\bar{1}}}{2}\,, \qquad \mathbf{T} = \frac{t_1 + t_{\bar{1}}}{2}\,, \qquad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_{\bar{1}}\,, \qquad \mathbf{t} = t_1 - t_{\bar{1}}$$

- $G^{<}(\mathbf{p}\omega, \mathbf{R}T)$ can be interpreted as the density of particles with momentum $\mathbf{p}$ and energy ω at the space time point $(\mathbf{R}, t)$
- Correspondingly, $G^{>}(\mathbf{p}\omega, \mathbf{R}T)$ denotes the density of states available to a particle that is added to the system at $(\mathbf{R}, t)$ with momentum $\mathbf{p}$ and energy ω

Spectral function $A(\omega)$ back

1. If the Hamiltonian is of single-particle type $\hat{H} = \sum_i \hat{H}^1(\mathbf{r}_i)$ (the eigenvalue problem can be solved) and the spectral function is given for (homogeneous systems) by

$$A(\mathbf{p}, \omega) = 2\pi\delta(\omega - E(\mathbf{p})) \,, \qquad E(\mathbf{p}) = \frac{p^2}{2m}$$

2. For (homogeneous) effective single-particle problems (e.g. in a Hartree-Fock theory) one can replace $E(\mathbf{p}) \rightarrow \frac{p^2}{2m} + \Delta(\mathbf{p})$, where $\Delta(\mathbf{p})$ are the corresponding self-energy contributions.

Time-dependent observables ◂ back

- More formally, one arrives at the general expression

$$\langle \hat{O} \rangle(t) = \frac{\mathrm{Tr}\left\{ T_{\mathscr{C}'} [\exp(-i \int_{\mathscr{C}'} d\bar{t}\, \hat{H}(\bar{t}))\, O(t)] \right\}}{\mathrm{Tr}\left\{ \hat{U}(t_0 - i\beta, t_0) \right\}} ,$$

where the exponential function is to be understood as Dyson series. $T_{\mathscr{C}'}$ is defined by

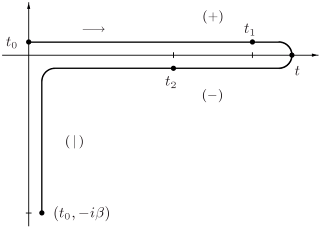
$$T_{\mathscr{C}'} \left(\hat{O}_1(t_1) \ldots \hat{O}_s(t_s) \right) = \sum_{\sigma \in \mathcal{P}_s} (\pm)^{I(\sigma)} \prod_{j=1}^{s-1} \theta(t_{\sigma_j}, t_{\sigma_{j+1}}) \prod_{k=1}^{s} \hat{O}_{\sigma_k}(t_{\sigma_k})$$

1. $T_{\mathscr{C}'}$ moves later operator to the left
2. Each exchange of two fermionic operators accompanied by a minus sign, i.e. $I(\sigma)$ gives the number of pair transpositions in permutation σ
3. $\theta(t_1, t_2) = 1$ if t_1 is situated later on the contour $\mathscr{C}'$ than t_2 and 0 otherwise

Full set of Green's functions ◂ back

In general: $G(1,\bar{1})$ can be understood as a 3×3-matrix of the form

$$\left(\begin{array}{cc|c} G^{++} & G^{+-} & G^{+|} \\ G^{-+} & G^{--} & G^{-|} \\ \hline G^{|+} & G^{|-} & G^{||} \end{array}\right) = \left(\begin{array}{cc|c} G^{c} & G^{<} & G^{\rceil} \\ G^{>} & G^{a} & G^{\rceil} \\ \hline G^{\lceil} & G^{\lceil} & G^{M} \end{array}\right)$$



- Correlation functions $G^{\gtrless}(1,\bar{1})$

$$G^{>}(1,\bar{1}) = \frac{1}{i}\left\langle \hat{\Psi}_H(1)\hat{\Psi}^{\dagger}_H(\bar{1})\right\rangle$$

$$G^{<}(1,\bar{1}) = \pm\frac{1}{i}\left\langle \hat{\Psi}^{\dagger}_H(\bar{1})\hat{\Psi}_H(1)\right\rangle$$

c: causal
a: anticausal

$$G^{c/a}(1,\bar{1}) = \theta(\pm[t_1 - t_{\bar{1}}])G^{>}(1,\bar{1}) + \theta(\pm[t_{\bar{1}} - t_1])G^{<}(1,\bar{1})$$

- Matsubara Green's function $G^M(1,\bar{1})$ with $\tau_1, \tau_{\bar{1}} \in \mathfrak{Im}\,\mathscr{C}'$

$$G^M(\mathbf{r}_1, \mathbf{r}_{\bar{1}}; \tau_1 - \tau_{\bar{1}}) = G(\mathbf{r}_1 t_0 - i\tau_1, \mathbf{r}_{\bar{1}} t_0 - i\tau_{\bar{1}})$$

- Mixed functions $G^{\lceil/\rceil}(1,\bar{1})$ with $t_1, t_{\bar{1}} \in \mathfrak{Re}\,\mathscr{C}'$ and $\tau_1, \tau_{\bar{1}} \in \mathfrak{Im}\,\mathscr{C}'$

$$G^{\rceil}(\mathbf{r}_1 t_1, \mathbf{r}_{\bar{1}}\tau_{\bar{1}}) = G^{<}(\mathbf{r}_1 t_1, \mathbf{r}_{\bar{1}} t_0 - i\tau_{\bar{1}})$$

$$G^{\lceil}(\mathbf{r}_1 \tau_1, \mathbf{r}_{\bar{1}} t_{\bar{1}}) = G^{>}(\mathbf{r}_1 t_0 - i\tau_1, \mathbf{r}_{\bar{1}} t_{\bar{1}})$$