Variational approaches beyond mean field

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+ in preparation

1. General construction of variational principles

$\{\mathcal{X}\} = \ldots \mathcal{X}^{\mu} \ldots$ $\begin{cases} \text{variables indexed by } \mu \\ \text{function of the variable } \mu \end{cases}$

Example: $\{\mathcal{X}\}$ = time-dependent ket $= |\xi(t)\rangle$ in Hilbert space

Physical value $\{X\}$ determined by equations

$$g^{\nu}\{\mathcal{X}\} = 0 \text{ , equivalent to } \{\mathcal{X}\} = \{X\}$$

Ex: g = Schrödinger equation (not exactly solvable)

Question: evaluate $\varphi = f\{\mathcal{X}\}$ for $\{\mathcal{X}\} = \{X\}$

Ex: φ = Scattering amplitude from $|\psi_i\rangle$ to $\langle\varphi_f|$:

$$f\{\mathcal{X}\} = \langle\varphi_f|\xi(t_f)\rangle \text{ for } |\xi(t_f)\rangle = |\psi(t_f)\rangle$$

Variational answer: regard $g^{\nu}\{\mathcal{X}\} = 0$ as constraints and introduce Lagrange multipliers (although we do not look for the maximum of $f\{\mathcal{X}\}$ for insufficient number of constraints)

Introduce function (or functional)

$$\Phi\{X,Y\} \equiv f\{X\} - \sum_\nu \underbrace{Y_\nu}_{\text{multipliers}} g^\nu\{X\}$$

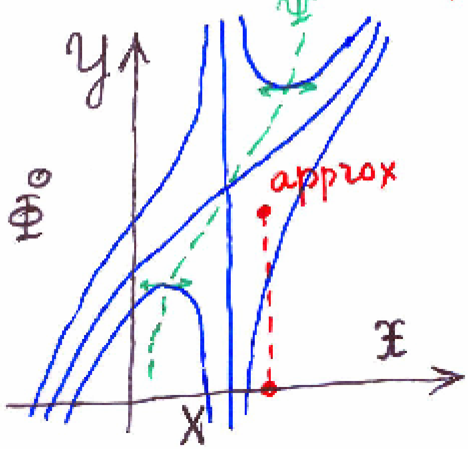
← Doubling the number of variables.

Then φ is the stationary value of Φ

Auxiliary stationarity conditions:

$$\frac{\partial f}{\partial X^\mu} - \sum_\nu Y_\nu \frac{\partial g^\nu}{\partial X^\mu} = 0$$

(useless for exact solution)



In restricted variational space, smaller error:

$$|f\{X^{ap}\} - f\{X\}| \gg |\Phi\{X^{ap}, Y^{ap}\} - \varphi|$$

$$-\sum Y \frac{\partial g}{\partial X}\Big|_{X^{ap}, Y^{ap}}$$

reduces the error.

Ex

$$\Phi\{|\xi(t)\rangle, \langle\eta(t)|\} = \overbrace{\langle\varphi_f|\xi(t_f)\rangle}^{f} - \int_{t_i}^{t_f} dt\, \underbrace{\langle\eta(t)|}_{Y}\, \underbrace{\frac{d}{dt} + iH\,|\xi(t)\rangle}_{g} \quad (k=1)$$

⇒ Lippmann-Schwinger

Auxiliary stationarity conditions:

$$\frac{d}{dt}\langle\eta(t)| - i\langle\eta(t)|H = 0, \quad \langle\eta(t_f)| = \langle\varphi_f|$$

= Backward Schrödinger eq.

Approximate eq. $\langle\delta\eta(t)|\frac{d}{dt} + iH|\xi(t)\rangle$ within allowed space.

$|\xi^{ap}(t)\rangle$ may depend on $\langle\varphi_f|$!!

Example 2 $\mathcal{X}$ = non-normalized density operator

$$\varphi = \underbrace{\ln \mathrm{Tr}\, X}_{f\{X\}} \quad , \quad \underbrace{X = e^{-\beta H}}$$

f not explicitly calculable

Constraint g: $\ln \mathcal{X} + \beta H = 0$

$$\Phi\{\mathcal{X}, \mathcal{Y}\} = \ln \mathrm{Tr}\, \mathcal{X} - \mathrm{Tr}\, \mathcal{Y}(\ln \mathcal{X} + \beta H)$$

Additional stationarity conditions:

$$\mathcal{Y} = \frac{\mathcal{X}}{\mathrm{Tr}\, \mathcal{X}}$$

- Elimination of half of the variables

$$\Psi\{\mathcal{Y}\} \equiv \Phi\{\mathcal{X}(\mathcal{Y}), \mathcal{Y}\}$$

$$= -\mathrm{Tr}\, \mathcal{Y} \ln \mathcal{Y} - \mathrm{Tr}\, \beta H \mathcal{Y} \quad (\mathrm{Tr}\, \mathcal{Y} = 1)$$

$\Rightarrow$ Minimization of the free energy $-\dfrac{\Psi}{\beta}$

Φ stationary, Ψ maximum

2. Generating functional

Questions: • Partition function

$$\mathrm{Tr}\, D \quad \text{for } D = e^{-\beta K}$$

• Expectation values at time t for given initial state $D(t_i)$

$$\langle Q_j(t)\rangle = \mathrm{Tr}\, Q_j^H(t,t_i) D(t_i) / \mathrm{Tr}\, D(t_i)$$

with $Q_j^H(t,t_i) = U^\dagger(t,t_i) Q_j^S U(t,t_i)$

• Correlation functions (any order)

$$C_{jk}(t',t'') = \mathrm{Tr}\, T Q_j^H(t',t_i) Q_k^H(t'',t_i) D(t_i) / \mathrm{Tr}\, D(t_i)$$

• Fluctuations

• Response functions

• Cross sections

Q_j = projection

All embedded in the characteristic functional

$$\Psi(\xi) \equiv \ln \mathrm{Tr}\, T\, e^{i\int_{t_i}^{\infty} dt' \sum_j \xi_j(t') Q_j^H(t',t_i)} D(t_i)$$

sources — observables of interest — initial state

through expansion in powers of the sources

$$\Psi(\xi) = \underline{\ln \operatorname{Tr} D(t_i)}$$ partition function (0)

$$+ i \sum_j \int_{t_i}^{\infty} dt' \, \xi_j(t') \, \underline{\langle Q_j(t') \rangle}$$ expectation values (1)

$$- \frac{1}{2} \sum_{jk} \iint_{t_i}^{\infty} dt' dt'' \, \xi_j(t') \xi_k(t'') \, \underline{C_{jk}(t', t'')}$$ correlations (2)

$$+ \ldots$$

Ingredients $\quad \Psi(\xi) = \ln \operatorname{Tr} A(t_i) D(t_i)$

- Generating operator

$$A(t) = T e^{i \int_t^{\infty} dt' \sum_j \xi_j(t') Q_j^H(t', t)}$$

Initial time t_i replaced by running time t !

- State $D(t_i)$ at initial time

$$D(t_i) = e^{-\beta K}$$

Possibly $\beta \to \infty$

Non equilibrium $K \neq H$ or $H - \mu N$

Look for variational principle for $\varphi \equiv \Psi(\xi)$

$$\{\mathcal{X}\} = \{\mathcal{A}(t), \mathcal{D}\}$$

Need workable equations $g\{\mathcal{X}\}$ to express that $\mathcal{A}(t) = A(t)$, $\mathcal{D} = D(t_i)$

in particular for $Q_j^H(t', t_i)$

3. Backward Heisenberg equation

- Standard (forward) Heisenberg equation

$$\frac{\partial U(t,t')}{\partial t} = -i H U(t,t')$$

$$\Rightarrow \quad \frac{dQ^H(t,t_i)}{dt} + i\left[Q^H(t,t_i), H\right] = 0$$

with $Q^H(t_i,t_i) = Q^S$

Shortcomings :

- If Q^S depends explicitly on time

$$\cdots = \left(\frac{\partial Q^S}{\partial t}\right)^H$$

requires new equation
... and so on

- If H depends explicitly on time

$(H)^H$ — Id —

- Anyhow Q^H hidden in $A(t)$!

- Backward : derivative / initial time

$$\frac{\partial U(t,t')}{\partial t'} = i\, U(t,t')\, H$$

$$\Rightarrow \quad \frac{dQ^H(t,t')}{dt'} - i\left[Q^H(t,t'), H\right] = 0$$

with $Q^H(t,t) = Q^S$

- No additional term if $Q^S(t)$
- $H = H^S(t')$ if explicit time-dependence

- Backward equation for $A(t)$

$$A(t) = T\, e^{i\int_t^\infty dt' \sum_j \xi_j(t')\, Q_j^H(t', t)}$$

$$* \quad \frac{dA(t)}{dt} - i\left[A(t), H\right] + i\, A(t) \sum_j \xi_j(t)\, Q_j^s = 0$$

to be solved, with $A(+\infty) = I$, backwards down to t_i.

Simple in spite of the complexity of $A(t)$ $(T, \exp, Q^H)$

4. Bloch equation

(Instead of constraint $\ln \mathcal{D} + \beta H = 0$)

Define $D(\tau) \equiv e^{-\tau K}$

$$\frac{dD(\tau)}{d\tau} + K\, D(\tau) = 0 \quad , \quad D(0) = I$$

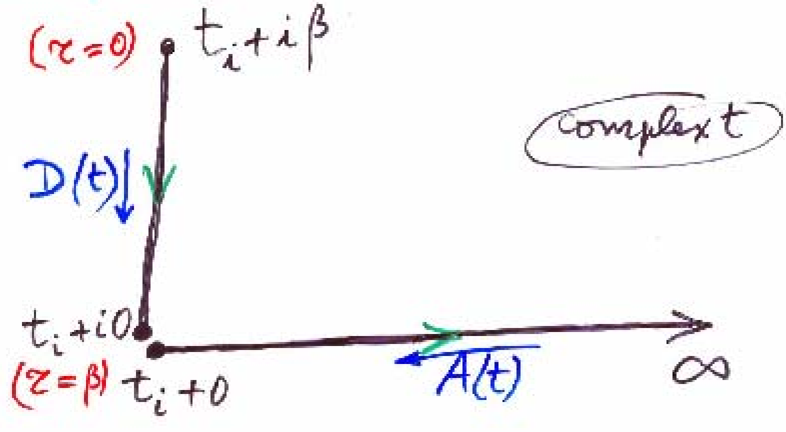
solution: $D(\beta) = \mathcal{D}(t_i)$

- Analogy with $A(t)$.

Made more complete with $\underline{t} = t_i + i(\beta - \underline{\tau})$

$$* \quad \frac{dD(t)}{dt} + i K\, D(t) = 0 \quad , \quad D(t_i + i\beta) = I$$

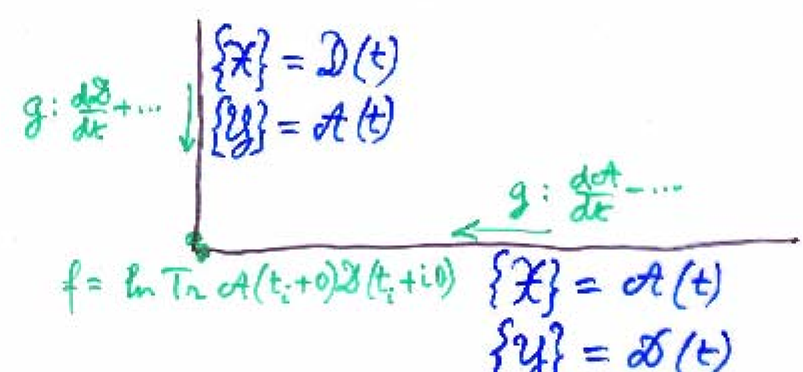
Integration contour



5. Variational principle for $\Psi(\xi)$

Merge: variat^{l} determination of (initial) state with Bloch eq. as constraint + variational determination of the dynamics through $dA(t)/dt$.

Variational parameters : time-dependent operators



$\Psi(\xi)$ = stationary value of

$$\boxed{\Phi\{x,y\} \equiv f\{x\} - \sum_\mu y_\mu \, g^\mu\{x\} \, w_\mu}$$

← possible weight

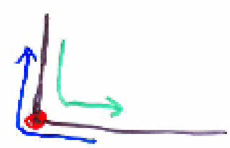
$$\Psi\{\mathcal{A}(t),\mathcal{D}(t)\} \equiv \ln \mathrm{Tr}\,\mathcal{A}(t_i+0)\,\mathcal{D}(t_i+i0)$$

$$-\int_{t_i+i\beta}^{t_i+i0} dt\, \mathrm{Tr}\,\mathcal{A}(t)\left(\frac{d\mathcal{D}}{dt}+iK\mathcal{D}(t)\right)\Big/\mathrm{Tr}\,\mathcal{A}(t)\mathcal{D}(t)$$

$$+\int_{t_i+0}^{+\infty} dt\,\mathrm{Tr}\,\mathcal{D}(t)\left(\frac{d\mathcal{A}}{dt} - i\left[\mathcal{A}(t),H\right] + i\mathcal{A}\sum_j \xi_j(t)\,Q^j\right)\Big/\mathrm{Tr}\,\mathcal{A}\mathcal{D}$$

with mixed boundary conditions $\mathcal{A}(+\infty)=I=\mathcal{D}(t_i+i\beta)$

Stationarity conditions / $\delta\mathcal{A}(t)$, $\delta\mathcal{D}(t)$

- Forward equations for $\mathcal{D}(t)$ on both parts of the contour 
- Backward equations for $\mathcal{A}(t)$
- Continuity at t_i of $\mathcal{D}$ and $\mathcal{A}$
- The source terms occur on the real branch only

Restricted trial spaces for $\mathcal{A}(t)$ and $\mathcal{D}(t)$ so that $\Psi\{\mathcal{A},\mathcal{D}\}$ be calculable

→ best estimate for $\Psi(\xi)$

The solution depends on the sources $\xi_j(t)$

Outcomes

implicit implicit explicit

$$\psi^{q}(\xi) = \Psi\left\{\mathcal{A}^{q}(\xi), \mathcal{D}^{q}(\xi), \xi\right\}$$

Expand : $\mathcal{A}^{q}(\xi) = \mathcal{A}^{(0)} + \mathcal{A}^{(1)} + \cdots$

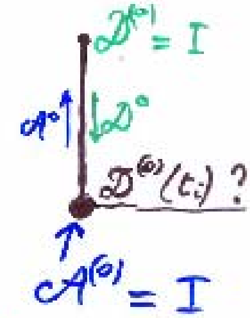
$\mathcal{D}^{q}(\xi) = \mathcal{D}^{(0)} + \mathcal{D}^{(1)} + \cdots$

- Zeroth order

Partition function $\psi(0) = \ln \operatorname{Tr} \mathcal{D}^{(0)}(t_i)$

Thermodynamics

$$\text{eqs.}\begin{cases} \operatorname{Tr} \delta\mathcal{A}^{(0)}(t)\left(\dfrac{d\mathcal{D}^{(0)}}{dt} + iK\mathcal{D}^{(0)}\right) = 0 \\ \operatorname{Tr} \delta\mathcal{D}^{(0)}(t)\left(\dfrac{d\mathcal{A}^{(0)}}{dt} - i\mathcal{A}^{(0)}K\right) = 0 \end{cases}$$



coupled if $\delta\mathcal{D}^{(0)}$ depends on $\mathcal{D}^{(0)}(t)$ in the chosen trial space

Example : Trial space = single-particle

$$\mathcal{D}(t) = \exp\left(\sum_{\mu\nu} J_{\mu\nu}\, a^{\dagger}_{\nu} a_{\mu}\right)$$

$\mathcal{A}(t)$ = idem

trial TD parameters

$\mathcal{D}^{(0)}(t_i)$ given by static Hartree-Fock theory

- First order

Requires only $\mathcal{D}^{(0)}$ and $\mathcal{A}^{(0)}$ due to stationarity

Expectation values [Q_j = energy, local density ...]

$$\langle Q_j(t)\rangle = -i\,\frac{\delta\Psi(\xi)}{\delta\xi_j(t)} \simeq \operatorname{Tr}\mathcal{D}^{(0)}(t)\,Q_j^s \,/\, \operatorname{Tr}\mathcal{D}^{(0)}$$

- at equilibrium

only $\mathcal{D}^{(0)}(t_i)$ as for thermodynamics

- off equilibrium, or $[Q_j^s, H] \neq 0$

$$\operatorname{Tr}\delta\mathcal{A}^{(0)}(t)\left(\frac{d\mathcal{D}^{(0)}}{dt} + i\left[H, \mathcal{D}^{(0)}(t)\right]\right) = 0$$

$\mathcal{D}^{(0)}(t_i) \longrightarrow \mathcal{D}^{(0)}(t)$?

time-dependent reduced Schrödinger eq. with initial condition variationally given by $\mathcal{D}^{(0)}(t_i)$.

Ex $\mathcal{D}^{(0)}(t)$ given by TDHF, with initial condition by static HF

Equivalent result in terms of $\mathcal{A}^{(1)}$ (although not needed!)

$$\mathcal{A}^{(1)}(t) \equiv i\sum_j \int_t^\infty dt'\,\xi_j(t')\,\underbrace{\mathcal{Q}_j(t',t)}$$

variational equivalent of $Q_j^H(t',t)$

$$\langle Q_j(t)\rangle = \operatorname{Tr}\mathcal{D}^{(0)}(t_i)\,\mathcal{Q}_j(t', t_i)$$

given by backward equation

$$\operatorname{Tr}\delta\mathcal{D}^{(0)}(t)\left(\frac{d\,\mathcal{Q}_j(t',t)}{dt} - i\left[\mathcal{Q}_j(t',t), H\right]\right) = 0$$

$$\mathcal{Q}_j(t',t') = Q_j^s$$

Heisenberg-like result

Ex Eq. for $Q_j(t',t)$ = <u>backward RPA</u> equation, recovered in a variational and unified framework

Two alternative equivalent expressions for $\langle Q_j(t)\rangle$

- Schrödinger-like, with $\mathcal{D}^{(0)}(t)$ TDHF
- Heisenberg-like, with $\mathcal{A}^{(1)}(t)$ backward RPA

plus in both cases $\mathcal{D}^{(0)}(t_i)$ static HF

- <u>Second order</u>: Correlations, fluctuations, linear responses

Requires (in general) $\mathcal{D}^{(1)}$ and $\mathcal{A}^{(1)}$ through

$$C_{jk}(t',t'') = -\frac{\delta\,\psi(\xi)}{\delta\xi_j(t')\,\delta\xi_k(t'')}$$

$\mathcal{D}^{(1)}$ depends on the observables under study! The approximation for the "state" $\mathcal{D}$ changes from one question to another, because $\mathcal{D}^{*}$ depends on ξ before expansion due to its coupling with $\mathcal{A}^{*}$.

→ $\mathcal{D}$ fitted to the question asked

→ Non-trivial results even with simple trial states: correlations with uncorrelated trial states!!

- Equilibrium correlations and fluctuations

$$C_{jk}(\pi_i, t_i) = \ldots.$$

Ex. Expressed in terms of the <u>static RPA</u> matrix

- Time-dependent correlations

Ex. Both static RPA to fit the initial state to the question asked, and backward RPA to simulate the dynamics of $Q_j^H(t'; t_i)$

Result simple only in the Heisenberg picture, not in the Schrödinger picture !

- Responses and dissipation

$$\chi_{jk}(t', t'') = -i\,\theta(t'-t'')\,\mathrm{Tr}\, D(t_i)\left[Q_j^H(t', t_i), Q_k^H(t'', t_i)\right]$$

$$\chi''_{jk}(\omega)$$

Variational expression involves only $\mathcal{D}^{(0)}$ although 2 operators Q

6. Trial spaces with group structure

Ex : $\mathcal{D} = \exp\left(\sum_{\mu\nu} J_{\mu\nu}\, a^\dagger_\nu a_\mu\right)$
independent particle operator
= Lie group with Lie algebra
of generators $M_\alpha \equiv a^\dagger_\nu a_\mu$

Many other examples : fermions with pairing ($a^\dagger a$, $a^\dagger a^\dagger$, aa), bosons with condensation ($a^\dagger a$, $a^\dagger a^\dagger$, aa, a, $a^\dagger$), spins ($\vec{\sigma}$).

Any Lie group

$$\mathcal{D} = \exp\left(J^\alpha M_\alpha\right) \qquad \mathcal{A} = \exp\left(L^\alpha M_\alpha\right)$$

M_α = Lie algebra : $[M_\alpha, M_\beta] = \Gamma^\gamma_{\alpha\beta} M_\gamma$
$M_0 = I$ included ($\mathcal{D}$ not normalized)

$\mathcal{D}\mathcal{A}$ also belongs to the group

Alternative parametrization

$$R_\alpha = \mathrm{Tr}\, M_\alpha \mathcal{D} \qquad \{R_\alpha\} \longleftrightarrow \{J^\alpha\}$$

Ex : $\rho_{\mu\nu} = \mathrm{Tr}\, a^\dagger_\mu a_\nu \mathcal{D}$ $\qquad \{\rho_{\mu\nu}\} \leftrightarrow \{J_{\mu\nu}\}$

Correspondence (depends on group structure):

$$R_\alpha = \frac{\partial}{\partial J^\alpha} \mathrm{Tr}\, \mathcal{D}\{J\}$$

$$J^\alpha = -\frac{\partial}{\partial R^\alpha} S\{R\} \qquad \text{(Legendre)}$$

$$S\{R\} = \mathrm{Tr}\,\mathcal{D} - \mathrm{Tr}\,\mathcal{D}\ln\mathcal{D} \qquad \text{Entropy}$$

Image of operators

$$Q \Rightarrow q\{R\} \equiv \mathrm{Tr}\, Q \mathcal{D} \quad (\text{generalizes } M_\alpha \Rightarrow R_\alpha)$$

$$H \Rightarrow h\{R\}$$ Hartree-Fock energy in terms of contractions $\rho_{\mu\nu}$

$$K \Rightarrow k\{R\} \quad \text{for } K = -\frac{1}{\beta} \ln D_{exact}(t_i)$$

Effective operators : correspondence from arbitrary Q to Q_{eff} in the Lie algebra

$$K_{eff} \equiv \frac{\partial k\{R\}}{\partial R_\alpha} M_\alpha$$ Hartree-Fock effective Hamiltonian (+ constant)

Properties :

$$\mathrm{Tr}\, \mathcal{D} K = \mathrm{Tr}\, \mathcal{D} K_{eff} = k\{R\}$$

$$\mathrm{Tr}\, \delta\mathcal{D} K = \mathrm{Tr}\, \delta\mathcal{D} K_{eff} = \frac{\partial k}{\partial R_\alpha} \delta R_\alpha$$

for variations in the group.

Useful matrices

$$\mathbb{H}^{\alpha\beta} = \frac{\partial^2 h}{\partial R_\alpha \partial R_\beta}, \quad \mathbb{K}^{\alpha\beta} = \frac{\partial^2 k}{\partial R_\alpha \partial R_\beta}, \quad \mathbb{S}^{\alpha\beta} = \frac{\partial^2 s}{\partial R_\alpha \partial R_\beta}$$

$$\mathbb{S}^{\alpha\beta} = -\frac{\partial J^\alpha}{\partial R_\beta}$$

$$dl^2 = -\delta R_\alpha \mathbb{S}^{\alpha\beta} \delta R_\beta$$

Natural metric in the space of states $\mathcal{D}$

$$\mathbb{C}_{\alpha\beta} = \mathrm{Tr}\, [M_\alpha, M_\beta] \mathcal{D}$$

$$= \Gamma^\gamma_{\alpha\beta} R_\gamma$$

$$\{\{R_\alpha, R_\beta\}\} = -i\, \mathbb{C}_{\alpha\beta}$$

Defines a Lie-Poisson structure in the space of "classical" variables $\{R\}$

[depends on $\{R\}$ $\neq$ Hamiltonian mechanics]

Outcomes

- Zeroth order (optimize partition functions $\mathrm{Tr}\,\mathcal{D}(t_i)$)

$$\ln \mathcal{D}^{(0)}(t_i) = -\beta K_{eff} \qquad \text{(in Lie algebra)}$$

or equivalently

$$S\{\mathcal{R}^{(0)}\} - \beta k\{\mathcal{R}^{(0)}\} \quad \text{maximum} \quad \text{(static HF)}$$

$\rightarrow$ self consistent equations

For $K = H$ or $H - \mu N$, all thermodynamic relations are satisfied (for canonical or grand canonical equilibrium) within replacement $K \Rightarrow K_{eff}$

- First order (optimize expectation values)

  - at t_i : $\langle Q_j \rangle = \mathrm{Tr}\, Q_j \mathcal{D}(t_i) = q_j\{\mathcal{R}^{(0)}(t_i)\}$
  - at t : $\langle Q_j(t) \rangle = q_j\{\mathcal{R}^{(0)}(t)\}$

$$\frac{d\mathcal{R}^{(0)}_\alpha}{dt} = -i\,\mathbb{C}_{\alpha\beta}\{\mathcal{R}^{(0)}\} \frac{\partial h\{\mathcal{R}^{(0)}(t)\}}{\partial \mathcal{R}^{(0)}_\beta(t)} \qquad \text{(TDHF)}$$

$$= -i\,\mathrm{Tr}\,\mathcal{D}^{(0)}(t)\,[\mathcal{R}^{(0)}_\alpha, H_{eff}] \quad \text{Ehrenfest}$$

$$= \{\{\mathcal{R}^{(0)}_\alpha(t), \underline{h\{\mathcal{R}^{(0)}(t)\}}\}\} \quad \text{"Classical" structure}$$

average energy = "Classical Hamiltonian" with Lie-Poisson bracket dynamics

Alternative expression in Heisenberg picture

$\mathcal{A}^{(1)}(t)$ belongs to the Lie algebra: define its coordinates $Q_j^\alpha(t',t)$ as

$$\mathcal{A}^{(1)}(t) = i\sum_j \int dt'\, \xi_j(t')\, \underbrace{Q_j^\alpha(t',t)\, M_\alpha}_{\equiv\, Q_j^H(t',t)_{\text{eff}}}$$

Then

$$\langle Q_j(t')\rangle = Q_j^\alpha(t',t_i)\, \mathcal{R}_\alpha^{(0)}(t_i)$$

$$= \mathrm{Tr}\ Q_j(t',t_i)\, \mathcal{D}^{(0)}(t_i)$$

Reduction of Heisenberg eq. in the group

Dynamics given by backward equation

$$\frac{d\, Q_j^\alpha(t',t)}{dt} = i\, Q_j^\gamma(t',t)\left[(\mathbb{C}\,\mathbb{H})_\gamma{}^\alpha + \Gamma_{\gamma\beta}^\alpha \frac{\partial h}{\partial R_\beta^{(0)}}\right]$$

Approx= for backward Heisenberg (Backward RPA)

- **Second order** (optimize correlations)

Determine $\mathcal{A}^{(1)}(t)$ and $\mathcal{D}^{(1)}(t)$ on the whole contour. Result:

$$C_{jk}(t',t'') = Q_j^\alpha(t',t_i)\, \underline{\mathbb{B}_{\alpha\beta}}\, \underline{Q_k^\gamma(t'',t_i)} \,/\, \mathrm{Tr}\,\mathcal{D}^{(0)}(t_i)$$

Depends on correction $\mathcal{D}^{(1)}(t_i)$ to initial state

Backward equation above

Explicit form:

$$\mathbb{F}^{\alpha\beta} = \frac{\partial^2}{\partial R_\alpha^{(0)}\, \partial R_\beta^{(0)}}\left[\underbrace{h\{R^{(0)}\} - \beta^{-1} s\{R^{(0)}\}}_{\text{Trial free energy}}\right]$$

$$\mathbb{B} = \frac{\mathbb{C}\,\mathbb{F}}{e^{\beta \mathbb{C}\mathbb{F}} - 1}\, \mathbb{F}^{-1}$$

(Static RPA)

Consistency properties

Not necessarily satisfied in naive approximations

- Conservation laws $[Q_j, H] = 0$ $\langle Q_j \rangle$ constant
- Simplifications for initial state at equilibrium

  $[K = H$ or $K = H - \mu N]$

→ $\langle Q_j(t) \rangle$ independent of t (HF = initial condition for TDHF)

→ $\langle Q_j(t') Q_k(t'') \rangle$ depends on $t = t' - t''$ only

non trivial but true!

Based on simplification of the approx^n for the backward Heisenberg equation:

$$\frac{d\mathcal{Q}_j^\alpha(t)}{dt} = -i\, \mathcal{Q}^\beta(t) (\mathbb{C}\mathbb{F})_\beta{}^\alpha$$

"Hamiltonian"

Not the same equation as for $\mathcal{R}^{(0)}(t)$!

$$\left(\frac{dR_\alpha^{(0)}(t)}{dt} = -i\, \mathbb{C}_{\alpha\beta} \frac{\partial h}{\partial R_\beta^{(0)}} \right)$$

Schrödinger picture

"Hamiltonian"

⇒ explicit solution for $\mathcal{Q}_j(t)$, replaced in C_{jk}:

$$C_{jk}(t) = \frac{1}{R_0^{(0)}} \frac{\partial q_j}{\partial R_\alpha^{(0)}}\, e^{-i\mathbb{C}\mathbb{F}t} \left(\frac{\mathbb{C}\mathbb{F}}{2} \coth \frac{\beta \mathbb{C}\mathbb{F}}{2}\, \mathbb{F}^{-1} \mp \frac{\mathbb{C}}{2} \right)_{\alpha\beta} \frac{\partial q_k}{\partial R_\beta^{(0)}}$$

$(t \gtrless 0)$

→ Response

$\chi_{jk}(t', t'')$ depends only on $t = t' - t''$

$$\chi_{jk}(t) = \frac{-i}{R_0^{(0)}}\theta(t)\frac{\partial q_j}{\partial R_\alpha^{(0)}}\left[e^{-i\mathbb{C}\mathbb{F}t}\mathbb{C}\right]_{\alpha\gamma}\frac{\partial q_k}{\partial R_\gamma^{(0)}}$$

→ Dissipation

$$\chi''_{jk}(\omega) = \frac{\pi}{R_0^{(0)}}\frac{\partial q_j}{\partial R_\alpha^{(0)}}\left[\delta(\hbar\omega - \mathbb{C}\mathbb{F})\mathbb{C}\right]_{\alpha\gamma}\frac{\partial q_k}{\partial R_\gamma^{(0)}}$$

Satisfy Kramers-Kronig relations

+ Fluctuation-dissipation theorem

- Vicinity of equilibrium

$$\frac{d\,\delta R_\alpha^{(0)}}{dt} = -i(\mathbb{C}\mathbb{F})_\alpha^{\ \beta}\,\delta R_\beta^{(0)} \quad \text{(For state)}$$

Same kernel as for backward equation for observable $\frac{d\mathcal{Q}^\alpha}{dt} = -i\,\mathcal{Q}^\beta(\mathbb{C}\mathbb{F})_\beta^{\ \alpha}$

Duality

Stability of equilibrium

- Eigenvalues of $\mathbb{C}\mathbb{F}$ real so that all modes of $\delta R_\alpha^{(0)}$ oscillatory
- Equivalence with the fact that equilibrium is given by the minimum of $\mathcal{F}\{\mathcal{R}\} \Rightarrow \mathbb{F}^{\alpha\beta}$ positive

7. Conclusion: flexibility of the method

- Restoration of broken invariances
- Density functional, and further