RPA
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Variational evaluation of fluctuations and correlations :

extensions of mean-field and RPA approaches

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RB + MV, Nuclear Phys. B 408 (1993) 445
RB, Hubert Flocard, MV, Phys. Reports 317 (1999) 251
RB + MV, paper hopefully achieved soon

- Outline of ideas pp 1-6
  Control variationally the optimization of approximations -
  Approximation of state depends on question asked
- General variational principle p 7
- An example of outcome pp 8-12

General but Formal ...!

Variational determination of correlations

RB + MV

Given state D at time t_i, evaluate approximately expectation values or correlation functions at t_i or later.

- Ex: delayed correlation between observables Q_j and Q_k, for initial state D:

$$C_{jk}(t',t'') \equiv \mathrm{Tr}\, \mathcal{T}\, Q_j^H(t',t_i)\, Q_k^H(t'',t_i)\, D - \langle Q_j^H(t',t_i)\rangle \langle Q_k^H(t'',t_i)\rangle ,$$

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

$$\frac{dU(t,t_i)}{dt} = -\frac{i}{\hbar} H\, U(t,t_i) .$$

Outcome: variational expression for C, involving RPA-type equations, used in a specific way.

- Other similar questions.

Synthesis of questions

Look for characteristic functional

$$\psi(\xi) \equiv \ln \mathrm{Tr}\, A(t_i) D .$$

→ Generating operator

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

Q_j : observables of interest,

$Q_j^H(t, t_i)$: Heisenberg representation,

$\xi_j(t)$: time-dependent sources.

→ State at time t_i

$$D = e^{-\beta K} .$$

- Equilibrium : g^d canonical $K = H - \mu N$.
  Non equilibrium : $[K, H] \neq 0$,
  e.g. boost for collisions.
- Non normalized D :
  e.g. $K = H$ provides $\psi(0) = \ln \mathrm{Tr}\, e^{-\beta H}$: thermodynamic potential
- Pure states treated as limit when $\beta \to \infty$.

Strategy : • optimize $\psi(\xi)$;
• expand in powers of ξ.

→ encompasses variational results for :

• Thermodynamic quantities (at zeroth order)

thermod. potential, entropy, level density
ground state energy

• Expectation values of selected observables (1st order)

time-dependent
$\mathrm{Tr}\, Q_j^H(t, t_i)\, \mathcal{D} \,/\, \mathrm{Tr}\, \mathcal{D}$
static

• Two-observable quantities (2nd order)

delayed correlations $C_{jk}(t', t'')$
correlations in state $\mathcal{D}$
fluctuations (time-dependent or not)
linear responses, dissipation

• Higher order correlations

Express ψ as the stationary value of some variational expression Ψ ?

- Write simple equations to characterize the ingredients $A(t_i)$ and D of ψ:

$$\psi = \ln \mathrm{Tr}\, A(t_i)\, D .$$

(replaced by trial objects $\mathcal{A}$ and $\mathcal{D}$)

- Treat these equations as constraints on the trial objects, to be satisfied approximately.
- Variational $\Psi\{\mathcal{A}, \mathcal{D}\}$ obtained by introducing Lagrange-like multipliers associated with the constraints.

$\Longrightarrow$ General method for constructing Ψ:

- based on doubling of the number of variables (ingredients + multipliers);
- then restrict their trial spaces.

Simple equation for generating operator

- Introduce auxiliary time t:

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

$$A(t_i) = \ldots (t_i) \ldots\ldots (t_i)$$

- Regard initial time t_i as running time t.

- Heisenberg operator

$$Q_j^H(t', t) = U^\dagger(t', t)\, Q_j^s\, U(t', t)$$

satisfies Heisenberg equation:

$$\frac{dQ_j^H(t', t)}{dt'} = -\frac{i}{\hbar}\left[Q_j^H(t', t), H^H(t')\right] + \left(\frac{\partial Q_j^s}{\partial t}\right)^H ,$$

and also simpler backward Heis^g equation:

$$\frac{dQ_j(t', t)}{dt} = \frac{i}{\hbar}\left[Q_j^H(t', t), H(t)\right]$$

in terms of the reference time.

- Yields for $A(t)$ the backward equation

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

Solution yields $A(t_i)$, with $A(\infty) = I$.

Unexpectedly simple !

Simple equation for state

$$D = e^{-\beta K}$$

- Bloch equation for $D(\tau) = e^{-\tau K}$

  depending again on auxiliary "time" τ:

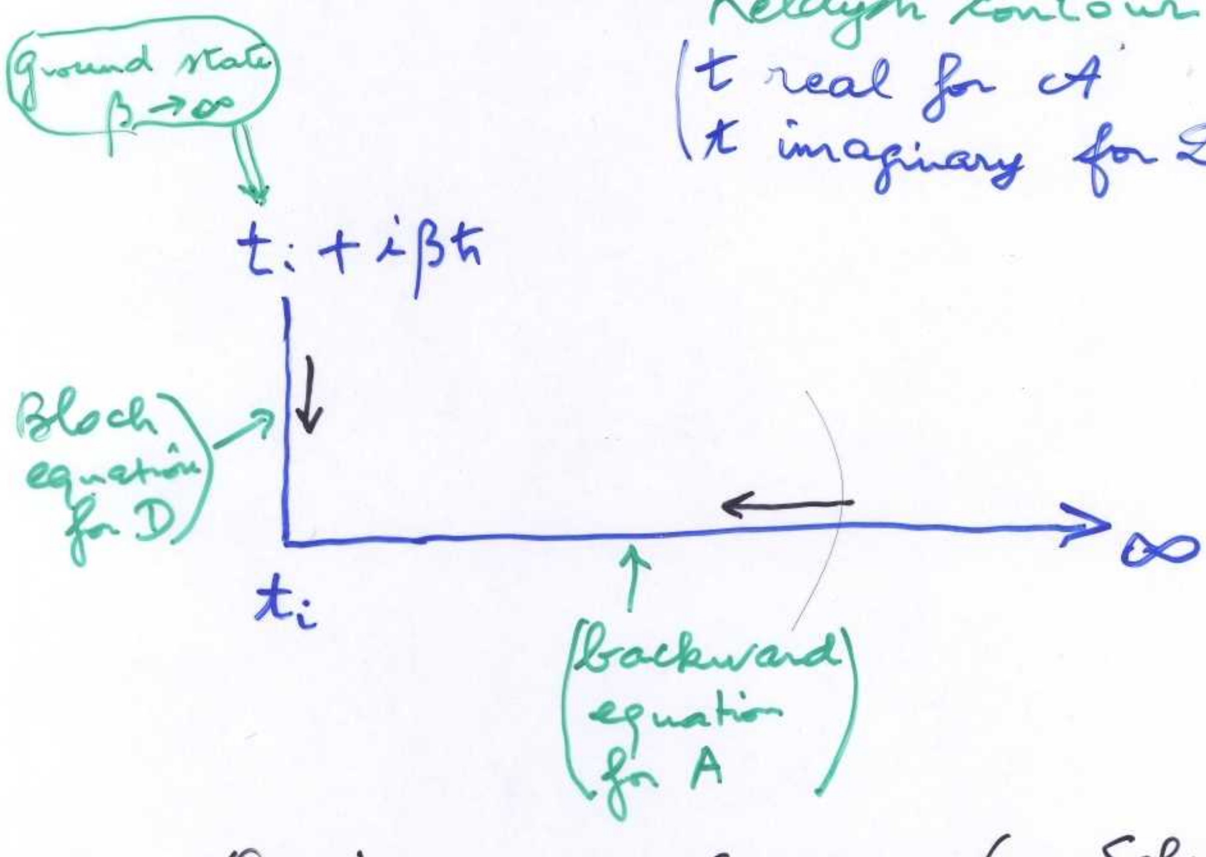
$$\frac{dD(\tau)}{d\tau} + K D(\tau) = 0$$

  yields $D = D(\tau = \beta)$ with $D(0) = I$.

- Replace τ by imaginary time

  → Keldysh contour.

  t real for $\mathcal{A}$
  t imaginary for $\mathcal{D}$



- Opposite arrows of time (~ Schwinger).

The characteristic functional $\Psi(\xi)$,

$$\Psi = \ln \mathrm{Tr}\, A(t_i)\, \mathcal{D},$$

is found as the stationary value of:

(line suppressed for static problems)

$$\Psi\{\mathcal{A}(t), \mathcal{D}(t)\} = \ln \mathrm{Tr}\, \mathcal{A}(t_\mathrm{i}+0)\mathcal{D}(t_\mathrm{i}+i0)$$

account for state $$- \int_{t_\mathrm{i}+i\beta\hbar}^{t_\mathrm{i}+i0} dt\, \mathrm{Tr}\, \mathcal{A}(t)\left[\frac{d\mathcal{D}(t)}{dt} + \frac{i}{\hbar} K\, \mathcal{D}(t)\right] [\mathrm{Tr}\, \mathcal{A}(t)\mathcal{D}(t)]^{-1}$$

account for dynamics $$+ \int_{t_\mathrm{i}+0}^{\infty} dt\, \mathrm{Tr}\left[\frac{d\mathcal{A}(t)}{dt} + \frac{1}{i\hbar}[\mathcal{A}(t), H] + i\,\mathcal{A}(t)\sum_j \xi_j(t)\, Q_j^{\mathrm{S}}\right] \mathcal{D}(t) [\mathrm{Tr}\, \mathcal{A}(t)\mathcal{D}(t)]^{-1}.$$

- Constraints (on Keldysh contour)
- Multipliers
- Data

Boundary conditions $\mathcal{D}(t_i + i\beta\hbar) = I$, $\mathcal{A}(\infty) = I$

(flexibility) → Use : Restrict trial space for operators $\mathcal{A}$ and $\mathcal{D}$

⇒ Var! equations $\delta\Psi = 0$. $\mathcal{D}$ depends on sources!

A family of variational approximations

- Trial space = Lie group.

  Example: $\mathcal{D}(t) = e^{\sum_{\mu\nu} J^{\mu\nu}(t) a^\dagger_\mu a_\nu}$

  independent-particle states

- *Generally*: $\mathcal{D}$ and $\mathcal{A}$ $\in$ Lie group generated by a Lie algebra $\{M\}$, parametrized as $\mathcal{D} = e^{J^\alpha M_\alpha}$.

  $\{M\} = \{a^\dagger_\mu a_\nu\}$, $\alpha = (\mu,\nu)$: ind^t particle Ansatz

  $\{M\} = \{a^\dagger_\mu a_\nu, a_\mu a_\nu, a^\dagger_\mu a^\dagger_\nu, I\}$: fermions with pairing

  $\{M\} = \{-\text{id}-, a_\mu, a^\dagger_\mu\}$: bosons with condens^{on}

  subalgebras .....

- Characterized by structure constants

$$[M_\alpha, M_\beta] = i\hbar\, \Gamma^\gamma_{\alpha\beta} M_\gamma .$$

- Workable is one can explicitly evaluate $\text{Tr}\, e^{J^\alpha M_\alpha}$ in terms of $\{J\}$.

- Alternative parametrization $\{R\} \Leftrightarrow \{J\}$

$$R_\alpha \equiv \frac{\text{Tr}\, M_\alpha \mathcal{D}}{\text{Tr}\, \mathcal{D}}$$

underlies all results.

For ind^t part^{les} $\{R\} = \rho_{\mu\nu} = \langle a^\dagger_\nu a_\mu \rangle$ in trial state

- Convenient tools to express the results
  - Image of an operator:

$$Q_j \Longleftrightarrow q_j\{R\} \equiv \frac{\mathrm{Tr}\, Q_j \mathcal{D}}{\mathrm{Tr}\, \mathcal{D}} .$$

= Representation by a scalar function depending on the set $\{R\}$ through $\mathcal{D}$

Likewise $h\{R\} \Leftrightarrow H$ (analogous to HF energy, but source dependent)

$k\{R\} \Leftrightarrow K$

also $S\{R\}$: entropy associated with $\mathcal{D}$

  - First derivatives of images

e.g. $\dfrac{\partial h}{\partial R_\alpha}$: change with $\mathcal{D}$ of the image h

(If H belongs to the Lie algebra, $M_\alpha \dfrac{\partial h}{\partial R_\alpha} = H$; otherwise $M_\alpha \dfrac{\partial h}{\partial R_\alpha} \equiv H_{eff}$ is an effective hamiltonian in the algebra)

  - Second derivatives of images: matrices

e.g. $\mathbb{H}^{\alpha\beta} \equiv \dfrac{\partial^2 h}{\partial R_\alpha \, \partial R_\beta}$, matrix in the α-space

Likewise $\mathbb{S}^{\alpha\beta}$.

Also $\mathbb{C}_{\alpha\beta} \equiv \Gamma^{\gamma}_{\alpha\beta} R_\gamma = \frac{1}{i\hbar} \mathrm{Tr}\left[M_\alpha, M_\beta\right]\mathcal{D}$

antisymmetric matrix

- Zeroth order in the sources

$$\psi(0) = \ln \mathrm{Tr}\, e^{-\beta K}$$

approached variationally by

$$\ln \mathrm{Tr}\, \mathcal{D}^{(0)} = \ln \mathrm{Tr}\, e^{-\beta K_{eff}\{R^\circ\}} = -\beta f\{R^\circ\},$$

where $\{R^\circ\}$ is defined by looking at the minimum of the trial free energy

$$f\{R\} = k\{R\} - \beta^{-1} S\{R\}$$

with respect to the parameters R of $\mathcal{D}$.

$\Rightarrow$ Self-consistent equations:

$$\beta \frac{\partial k}{\partial R^\circ_\alpha} = \frac{\partial S}{\partial R^\circ_\alpha}$$

- Moreover, the matrix $\mathbb{F}^{\alpha\beta}$ is positive.

(indep^t particle example $\Rightarrow$ Static HF eq)

- First order

  - Expectation values at $t = t_i$:

$$\langle Q_j(0) \rangle = q_j\{R^\circ\} \qquad \text{(static HF)}$$

  - Expectation values depending on time:

$$\langle Q_j(t) \rangle = q_j\{R^\circ(t)\}$$

with $\{R^\circ(t)\}$ given variationally by

$$\frac{dR^\circ_\alpha(t)}{dt} = \mathbb{C}_{\alpha\beta}\{R^\circ(t)\} \frac{\partial h}{\partial R^\circ_\beta} . \qquad \text{(TDHF)}$$

NB : Quantum approximate equation, with a classical Poisson structure (canonical parametrizations of $\{R\}$)

- Evolution of small deviations:

$$\boxed{\frac{d\,\delta R^{\circ}_{\alpha}}{dt} = (\mathbb{C}\mathbb{H} + \mathbb{T})_{\alpha}^{\beta}\,\delta R^{\circ}_{\beta}},$$

$$\mathbb{T}_{\alpha}^{\beta} = \Gamma_{\alpha\gamma}^{\beta}\,\frac{\partial h}{\partial R^{\circ}_{\gamma}}.$$

(Time-dependent RPA equation)

- Alternative expression of $\langle Q_j(t)\rangle$: in terms of the variational approximation for $Q_j^H(t',t)$, $\mathcal{Q}_j^H(t',t) = \mathcal{Q}_j^{\alpha}(t',t)\,M_{\alpha}$.

$$\left[\langle Q_j(t')\rangle \simeq \langle \mathcal{Q}_j^H(t',t_i)\rangle = \mathcal{Q}_j^{\alpha}(t',t_i)\,R^{\circ}_{\alpha}.\right.$$

Given by approximate backward Heisenberg eq.

$$\left[\frac{d\,\mathcal{Q}_j^{\alpha}(t',t)}{dt} = -\,\mathcal{Q}_j^{\beta}(t',t)\,(\mathbb{C}\mathbb{H} + \mathbb{T})_{\beta}^{\alpha}\right.$$

(dual kernel)

(Backward time-dep.t RPA eq.)

- Second order (main new result!)

- Delayed correlation function $(t' \geq t'')$:

$$\left[C_{jk}(t',t'') = \mathcal{Q}_j^{\alpha}(t',t_i)\,\mathbb{B}_{\alpha\gamma}\,\mathcal{Q}_k^{\gamma}(t'',t_i).\right.$$

Time dependence through approximate backward Heisenberg eq. with boundary condition $\mathcal{Q}_j^{\alpha}(t',t'-0) = \frac{\partial}{\partial R^{\circ}_{\alpha}(t')}\,q\{R^{\circ}(t')\}$

(Backward t-d. RPA)

$$\mathbb{B} = \left[\tfrac{1}{2} i\hbar\, \mathbb{C}\mathbb{F} \coth\left(\tfrac{1}{2} i\hbar \beta \mathbb{C}\mathbb{F}\right)\right]\mathbb{F}^{-1} + \frac{1}{2} i\hbar\, \mathbb{C}$$

$\mathbb{B}_{\alpha\beta}$ = var[l] approximation for correlation $\langle M_\alpha M_\beta \rangle - \langle M_\alpha \rangle \langle M_\beta \rangle$ in state D

$$\begin{cases} \mathbb{C}_{\alpha\beta} = \Gamma^{\gamma}_{\alpha\beta} R^{\circ}_{\gamma} \\ \mathbb{F}_{\alpha\beta} = \dfrac{\partial^2}{\partial R^{\circ}_{\alpha} \partial R^{\circ}_{\beta}} \left[k\{R^{\circ}\} - \beta^{-1} S\{R^{\circ}\} \right] \end{cases}$$

($\mathbb{C}\mathbb{F}$ = static RPA kernel)

- Special cases: equal time correlations, fluctuations, linear responses, dissipation.
- For initial state at equilibrium, $K = H$, the kernel of dynamical eq. simplifies as $\mathbb{C}\mathbb{H} + \mathbb{T} = \mathbb{C}\mathbb{F}$, so that

$$C_{jk}(t', t'') = \frac{\partial q_j}{\partial R^{\circ}_{\alpha}} \left[e^{(t'-t'')\mathbb{C}\mathbb{F}} \mathbb{B} \right]_{\alpha\gamma} \frac{\partial q_k}{\partial R^{\circ}_{\gamma}}$$

- Consistency properties

  $C_{jk}(t' - t'')$ Conservation laws

  Kramers-Kronig Kubo (fluct-diss[=])

- Static stability of eq. $\mathbb{F} \geq 0$ implies reality of eigenvalues of the kernel $i\mathbb{C}\mathbb{F}$ = dynamic stability

  (Thouless theorem)