CISS07 8/31/2007

Comprehensive treatment of correlations at different energy scales in nuclei using Green's functions

Lecture 1: 8/28/07	Propagator description of single-particle motion and the link with experimental data
Lecture 2: 8/29/07	From Hartree-Fock to spectroscopic factors < 1: inclusion of long-range correlations
Lecture 3: 8/29/07	Role of short-range and tensor correlations associated with realistic interactions
Lecture 4: 8/30/07	Dispersive optical model and predictions for nuclei towards the dripline
Adv. Lecture 1: 8/30/07	Saturation problem of nuclear matter & pairing in nuclear and neutron matter
Adv. Lecture 2: 8/31/07	Quasi-particle density functional theory

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Quasiparticle density functional theory QPDFT

Van Neck et al. Phys. Rev. A74, 042501(2006)

- Kohn-Sham implementation of density functional theory “as simple” as Hartree-Fock but includes correlations beyond HF while still only solving sp equations (self-consistently)
- DFT not good for near degenerate systems characterized by small particle-hole gaps
- Wave functions not easily interpreted
- Quasiparticles (QPs) are missing from KS-DFT
- Near the Fermi energy QPs describe the physics (Landau)

Motivation ⇒

- Develop sp equations whose solutions correspond to QP orbitals and energies, including the total energy and density matrix of the system (QPDFT) Dimitri Van Neck, U of Ghent

New framework to do self-consistent sp theory

Quasiparticle density functional theory ⇒ QP-DFT

D. Van Neck et al., Phys. Rev. A**74**, 042501 (2006)

Ground-state energy and one-body density matrix from self-consistent sp equations that extend the Kohn-Sham scheme.

Based on separating the propagator into a quasiparticle part and a background, expressing only the latter as a functional of the density matrix.

⇒ in addition yields qp energies and overlap functions

Reminder: DFT does not yield removal energies of atoms

Relative deviation [%]

		DFT	HF
He atom	1s	37.4	1.5
Ne atom	2p	38.7	6.8
Ar atom	3p	36.1	2.0

While ground-state energies are closer to exp in DFT than in HF

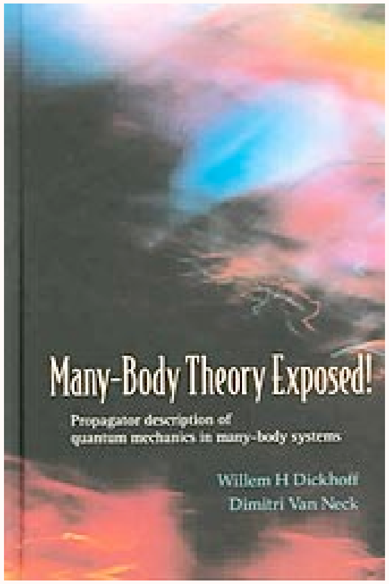
Can be developed for nuclei from DOM input!

Description of the nuclear many-body problem

Ingredients: Nucleons interacting by "realistic interactions"
Nonrelativistic many-body problem

Method: Green's functions (Propagators)
⇨ amplitudes instead of wave functions
keep track of all nucleons, including the high-momentum ones

Book:



Dimitri Van Neck & W.D.

Review: W.D. & C. Barbieri, Prog. Part. Nucl. Phys. **52**, 377 (2004)

Lecture notes: http://www.nscl.msu.edu/~brown/theory-group/lecture-notes.html

Single-particle propagator in the medium

Definition $$G(\alpha,\beta;t-t') = -\frac{i}{\hbar}\left\langle \Psi_0^N \middle| T\left[a_{\alpha_H}(t)\,a^\dagger_{\beta_H}(t')\right] \middle| \Psi_0^N \right\rangle$$

with $$\hat{H}\left|\Psi_0^N\right\rangle = E_0^N\left|\Psi_0^N\right\rangle$$ for the exact ground state

and $$a_{\alpha_H}(t) = e^{\frac{i}{\hbar}\hat{H}t}\,a_\alpha\,e^{-\frac{i}{\hbar}\hat{H}t}$$ (Heisenberg picture)

while *T* orders the operators with larger time on the left including a sign change

$$G(\alpha,\beta;t-t') = -\frac{i}{\hbar}\Big\{\theta(t-t')\,e^{\frac{i}{\hbar}E_0^N(t-t')}\left\langle \Psi_0^N \middle| a_\alpha e^{-\frac{i}{\hbar}\hat{H}(t-t')} a^\dagger_\beta \middle| \Psi_0^N \right\rangle$$ particle

$$-\,\theta(t-t')\,e^{\frac{i}{\hbar}E_0^N(t'-t)}\left\langle \Psi_0^N \middle| a^\dagger_\beta e^{-\frac{i}{\hbar}\hat{H}(t'-t)} a_\alpha \middle| \Psi_0^N \right\rangle\Big\}$$ hole

Fourier transform of G (Lehmann representation)

$$G(\alpha,\beta;E) = \left\langle \Psi_0^N \right| a_\alpha \frac{1}{E-\left(\hat{H}-E_0^N\right)+i\eta} a_\beta^\dagger \left| \Psi_0^N \right\rangle \quad \Leftarrow \text{Particle part}$$

$$+\left\langle \Psi_0^N \right| a_\beta^\dagger \frac{1}{E+\left(\hat{H}-E_0^N\right)-i\eta} a_\alpha \left| \Psi_0^N \right\rangle \quad \Leftarrow \text{Hole part}$$

$$= \sum_n \frac{\left\langle \Psi_0^N \right| a_\alpha \left| \Psi_n^{N+1} \right\rangle \left\langle \Psi_n^{N+1} \right| a_\beta^\dagger \left| \Psi_0^N \right\rangle}{E-\left(E_n^{N+1}-E_0^N\right)+i\eta} + \sum_n \frac{\left\langle \Psi_0^N \right| a_\beta^\dagger \left| \Psi_n^{N-1} \right\rangle \left\langle \Psi_n^{N-1} \right| a_\alpha \left| \Psi_0^N \right\rangle}{E+\left(E_n^{N-1}-E_0^N\right)-i\eta}$$

$$= \sum_n \frac{\left(z_n^{(+)}\right)_\alpha \left(z_n^{(+)}\right)_\beta^*}{E-\varepsilon_n^{(+)}+i\eta} + \sum_n \frac{\left(z_n^{(-)}\right)_\alpha \left(z_n^{(-)}\right)_\beta^*}{E-\varepsilon_n^{(-)}-i\eta}$$

Poles $\varepsilon_n^{(+)}$ in addition domain $\left(\varepsilon_0^{(+)},+\infty\right)$

Poles $\varepsilon_n^{(-)}$ in addition domain $\left(-\infty,\varepsilon_0^{(-)}\right)$

Finite systems particle-hole gap

$$\varepsilon_0^{(+)} - \varepsilon_0^{(-)} = E_0^{N+1} - 2E_0^{N} + E_0^{N-1} > 0$$

"Fermi energy" $\varepsilon_F = \frac{1}{2}\left(\varepsilon_0^{(+)} + \varepsilon_0^{(-)}\right) = \frac{1}{2}\left(E_0^{N+1} - E_0^{N-1}\right)$

Numerator contains information about "wave functions"

$$\left(z_n^{(-)}\right)_\alpha = \left\langle \Psi_n^{N-1} \middle| a_\alpha \middle| \Psi_0^N \right\rangle \quad \text{and} \quad \left(z_n^{(+)}\right)_\beta^* = \left\langle \Psi_m^{N+1} \middle| a_\beta^\dagger \middle| \Psi_0^N \right\rangle$$

while denominator identifies eigenvalues of H for the $N\pm1$ states

Note $$\hat{H}\left|\Psi_n^{N\pm1}\right\rangle = E_n^{N\pm1}\left|\Psi_n^{N\pm1}\right\rangle$$

has been used for exact $N \pm 1$ states of H

Density and Removal Energy Matrices

One-body density matrix

$$N^{(-)}_{\alpha,\beta} = \int \frac{dE}{2\pi i} e^{i\eta E} G(\alpha,\beta;E) = \sum_n \left(z_n^{(-)}\right)_\alpha \left(z_n^{(-)}\right)^*_\beta = \left\langle \Psi_0^N \left| a^\dagger_\beta a_\alpha \right| \Psi_0^N \right\rangle$$

Removal energy matrix

$$M^{(-)}_{\alpha,\beta} = \int \frac{dE}{2\pi i} e^{i\eta E} E\; G(\alpha,\beta;E) = \sum_n \varepsilon_n^{(-)} \left(z_n^{(-)}\right)_\alpha \left(z_n^{(-)}\right)^*_\beta = \left\langle \Psi_0^N \left| a^\dagger_\beta \left[a_\alpha, \hat{H}\right] \right| \Psi_0^N \right\rangle$$

Removal part of propagator yields any one-body observable plus

$$E_0^N = \frac{1}{2} Tr\left(\left[H_0\right]\left[N^{(-)}\right] + \left[M^{(-)}\right]\right)$$ the total energy (Migdal-Galitskii)

Eigenvalue problem in finite systems

Dyson equation reads $\left[G(E)\right]^{-1} = \left[G_0(E)\right]^{-1} - \left[\Sigma(E)\right]$

includes noninteracting propagator and self-energy.
Self-energy acts as an energy-dependent sp potential.
For discrete poles of the propagator

$$\left(\left[H_0\right] + \left[\Sigma\left(\varepsilon_n^{(\pm)}\right)\right]\right) z_n^{(\pm)} = \varepsilon_n^{(\pm)} z_n^{(\pm)}$$

acts in single-particle space

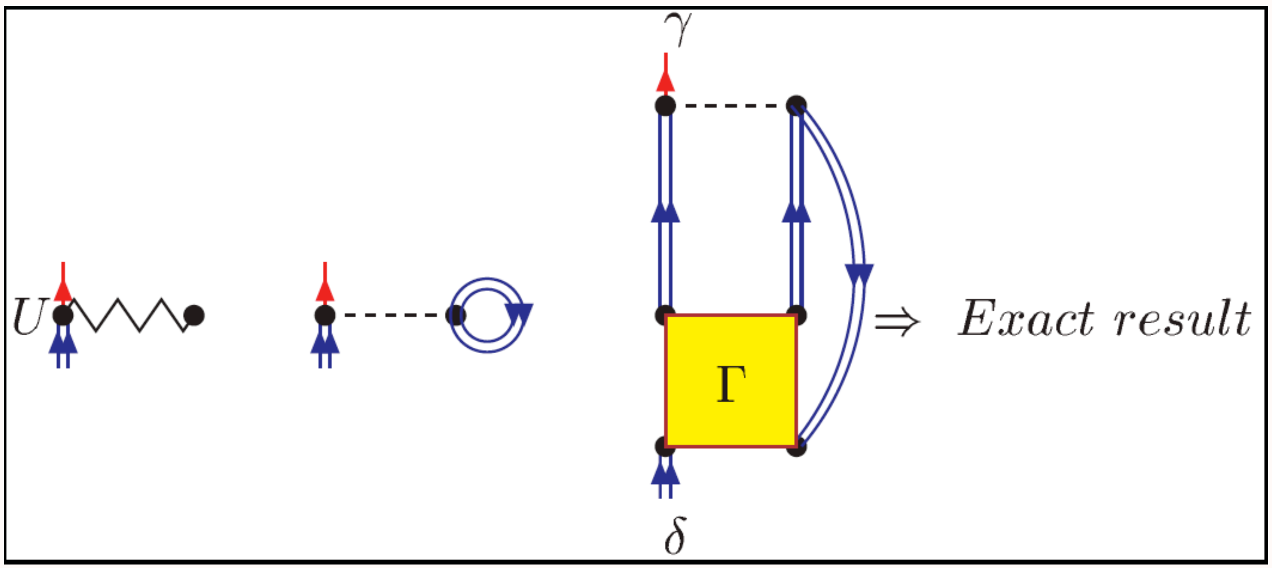
Dyson equation and vertex function

Fourier transform of equation of motion for *G* yields again the Dyson equation with the self-energy

$$\Sigma^*(\gamma,\delta;E) = -\langle\gamma|U|\delta\rangle - i\int_{C\uparrow}\frac{dE'}{2\pi}\sum_{\mu\nu}\langle\gamma\mu|V|\delta\nu\rangle G(\nu,\mu;E')$$

$$+\frac{1}{2}\int\frac{dE_1}{2\pi}\int\frac{dE_2}{2\pi}\sum_{\varepsilon\mu\nu\zeta\rho\sigma}\langle\gamma\mu|V|\varepsilon\nu\rangle G(\varepsilon,\zeta;E_1)G(\nu,\rho;E_2)G(\sigma,\mu;E_1+E_2-E)\langle\zeta\rho|\Gamma(E_1,E_2;E)|\delta\sigma\rangle$$

In diagram form



Spectral function

Single-particle spectral function

$$[S(E)] = \frac{1}{2\pi i} sign(\varepsilon_F - E)\left([G(E)] - [G(E)]^\dagger\right)$$

$$= \sum_n \left(z_n^{(+)}\right)\left(z_n^{(+)}\right)^\dagger \delta\left(E - \varepsilon_n^{(+)}\right) + \sum_n \left(z_n^{(-)}\right)\left(z_n^{(-)}\right)^\dagger \delta\left(E - \varepsilon_n^{(-)}\right)$$

Sum rules

$$N_{\alpha,\beta} = \int_{-\infty}^{+\infty} dE\ S(\alpha,\beta;E) = \left\langle \Psi_0^N \left| \left\{ a_\beta^\dagger, a_\alpha \right\} \right| \Psi_0^N \right\rangle$$

$$M_{\alpha,\beta} = \int_{-\infty}^{+\infty} dE\ E\ S(\alpha,\beta;E) = \left\langle \Psi_0^N \left| \left\{ a_\beta^\dagger, \left[a_\alpha, \hat{H} \right] \right\} \right| \Psi_0^N \right\rangle$$

Integrations over the entire energy axis

Split integration

$$N_{\alpha,\beta} = \int_{-\infty}^{\varepsilon_F} dE\ S(\alpha,\beta;E) + \int_{\varepsilon_F}^{+\infty} dE\ S(\alpha,\beta;E) = N_{\alpha,\beta}^{(-)} + N_{\alpha,\beta}^{(+)}$$

and similarly for

$$M_{\alpha,\beta} = \int_{-\infty}^{\varepsilon_F} dE\ E\ S(\alpha,\beta;E) + \int_{\varepsilon_F}^{+\infty} dE\ E\ S(\alpha,\beta;E) = M_{\alpha,\beta}^{(-)} + M_{\alpha,\beta}^{(+)}$$

Evaluating (anti)commutators (previous slide) sum rule can be written in closed form

$$N_{\alpha,\beta} = \delta_{\alpha,\beta} \quad \text{or} \quad [N] = [I]$$

and $$M_{\alpha,\beta} = \langle\alpha|H_0|\beta\rangle + \sum_{\gamma\delta} \langle\alpha\gamma|V|\beta\delta\rangle N_{\delta\gamma}^{(-)} \quad \text{or} \quad [M] = [H_0] + [\tilde{V}_{HF}]$$

Quasiparticles

Simple-minded form is modification of noninteracting propagator

$$G_Q(\alpha,\beta;E) = \sum_{j=1}^{N} \frac{\left(z_{Qj}\right)_\alpha \left(z_{Qj}\right)_\beta^*}{E - \varepsilon_{Qj} - iw_{Qj}} + \sum_{j=N+1}^{\infty} \frac{\left(z_{Qj}\right)_\alpha \left(z_{Qj}\right)_\beta^*}{E - \varepsilon_{Qj} + iw_{Qj}}$$

with widths > 0 and corresponding qp orbits and energies.
First term corresponds to excitations in the (N-1)-particle system with QP energies < the Fermi energy.
Corresponding spectral function

$$\left[S_Q(E)\right] = \sum_{j=1}^{\infty} \left(z_{Qj}\right)\left(z_{Qj}\right)^\dagger £_{w_{Qj}}\left(E - \varepsilon_{Qj}\right)$$

with $$£_\Delta(x) = \frac{1}{\pi}\frac{\Delta}{x^2 + \Delta^2}$$

QP properties

- Set of QP orbitals is complete and linearly independent but in general not orthogonal.
- QP ≠ HF because terms beyond lowest order are included
- Energy-dependent part of self-energy reduces spectroscopic strength

$$z_{Qj}^{\dagger} z_{Qj} \leq 1$$

- Interpretation "clear" in atoms and nuclei near the Fermi energy

QP contribution to sum rules

$$\left[N_Q\right] = \sum_{j=1}^{\infty} z_{Qj} z_{Qj}^{\dagger} \qquad *$$

$$\left[M_Q\right] = \sum_{j=1}^{\infty} \varepsilon_{Qj} z_{Qj} z_{Qj}^{\dagger} \qquad **$$

QP width does not contribute to 0th and 1st moment! Forget about it!

General statements

Given arbitrary Hermitian matrices $\left[N_Q\right]$ and $\left[M_Q\right]$ with $\left[N_Q\right]$ positive definite, one can obtain a unique decomposition of * and ** by solving the generalized eigenvalue problem

$$\left[M_Q\right]u_j = \lambda_j\left[N_Q\right]u_j$$

$$u_j^\dagger\left[N_Q\right]u_k = \delta_{j,k}$$

where $\left[N_Q\right]$ plays the role of a metric matrix.

So QP energies and orbitals are given by $\varepsilon_{Qj} = \lambda_j$

$$z_{Qj} = \left[N_Q\right]u_j$$

Use only ε_Q & z_Q, since widths extend strength beyond ε_F

QP contribution to density and removal energy matrices

$$\left[N_Q^{(-)}\right] = \sum_{j=1}^{N} z_{Qj} z_{Qj}^{\dagger}$$

$$\left[M_Q^{(-)}\right] = \sum_{j=1}^{N} \varepsilon_{Qj} z_{Qj} z_{Qj}^{\dagger}$$

and similarly for

$$\left[N_Q^{(+)}\right] = \sum_{j=N+1}^{\infty} z_{Qj} z_{Qj}^{\dagger}$$

$$\left[M_Q^{(+)}\right] = \sum_{j=N+1}^{\infty} \varepsilon_{Qj} z_{Qj} z_{Qj}^{\dagger}$$

QP equations

QP contribution to spectral function dominant so isolate it

$$\left[S(E)\right] = \left[S_Q(E)\right] + \left[S_B(E)\right]$$

defining the background contribution.
Full energy dependence of S_B not needed, since

$$\left[N\right] = \left[N_Q\right] + \left[N_B\right]$$

$$\left[M\right] = \left[M_Q\right] + \left[M_B\right]$$

Left sides known!!
(see earlier slide)

Where total energy integrals can be split into removal and addition part

$$\left[N_B\right] = \left[N_B^{(-)}\right] + \left[N_B^{(+)}\right]$$

$$\left[M_B\right] = \left[M_B^{(-)}\right] + \left[M_B^{(+)}\right]$$

Main result

Remarkable conclusion: modeling background contributions

$\left[M_B^{\pm}\right]$

$\left[N_B^{\pm}\right]$

as a functional of the density matrix $\left[N^{(-)}\right]$

is sufficient to generate a self-consistent set of sp equations.
Rewriting eigenvalue problem generates

$$\left(\left[H_0\right]+\left[\tilde{V}_{HF}\left\{N^{(-)}\right\}\right]-\left[M_B\left\{N^{(-)}\right\}\right]\right)u_j = \lambda_j\left(\left[I\right]-\left[N_B\left\{N^{(-)}\right\}\right]\right)u_j$$

Initial estimate for $\left[N^{(-)}\right]$ allows construction of $\left[N_B\right]$ and $\left[M_B\right]$
but also $\left[\tilde{V}_{HF}\right]$

Procedure

$$\left(\left[H_0\right]+\left[\tilde{V}_{HF}\left\{N^{(-)}\right\}\right]-\left[M_B\left\{N^{(-)}\right\}\right]\right)u_j=\lambda_j\left(\left[I\right]-\left[N_B\left\{N^{(-)}\right\}\right]\right)u_j$$

Then eigenvalue problem can be solved yielding

QP energies

$$\varepsilon_{Qj}=\lambda_j$$

and QP orbits

$$z_{Qj}=\left(\left[I\right]-\left[N_B\left\{N^{(-)}\right\}\right]\right)u_j$$

N lowest energy solutions belong in *N*-1 and can be used to update the density matrix

$$\left[N_{new}^{(-)}\right]=\sum_{j=1}^{N}z_{Qj}z_{Qj}^{\dagger}+\left[N_B^{(-)}\left\{N^{(-)}\right\}\right]$$

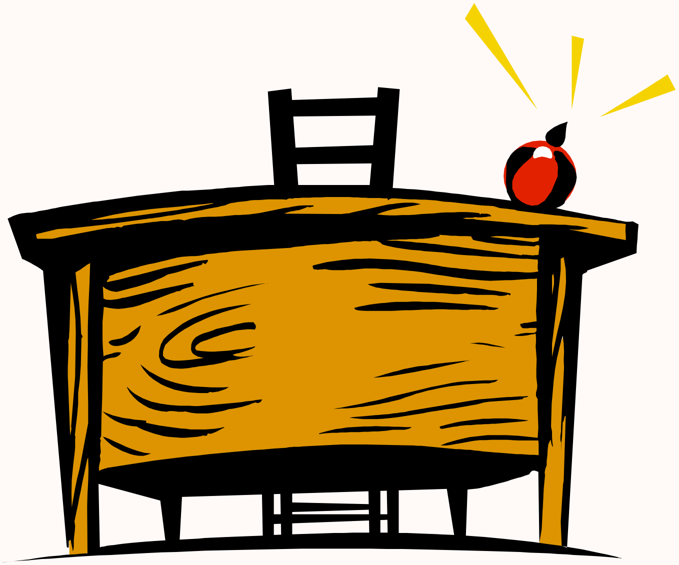
closing the self-consistency loop!

Total energy follows from

$$E_0^N=\frac{1}{2}\sum_{j=1}^{N}z_{Qj}^{\dagger}\left(\left[H_0\right]+\varepsilon_{Qj}\right)z_{Qj}+\frac{1}{2}Tr\left(\left[H_0\right]\left[N_B^{(-)}\left\{N^{(-)}\right\}\right]+\left[M_B^{(-)}\left\{N^{(-)}\right\}\right]\right)$$

Comments

- Formalism generates total energy, density matrix, and individual QP energies and orbits (with correct spectroscopic factors) starting from a model for the background contributions [$M_B^{(\pm)}$] and [$N_B^{(\pm)}$] as a functional of the density matrix.
- M_B plays different role in nuclear systems as compared to electronic systems (responsible for attraction that binds system)
- Recent work on modeling the complete nucleon self-energy (Charity *et al.*) provides information to generate functionals near and at intermediate energies from the Fermi energy
- Self-energy from nuclear matter provides this information for energies far away, including the effect of short-range correlations
- Intermediate implementations are possible $\Rightarrow$ adapt Skyrme functional approach
- Formalism includes HF and KS-DFT (see Van Neck paper)



Time to stop!

Thanks for listening