GREEN FUNCTION INTERPRETATION OF BRUECKNER THEORY

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ABSTRACT: The basic features of Hartree-Fock theory are the presence of a single-particle hermitean common potential well operator and the associated spectrum of (real) energies and orbitals. The need for a renormalized Hartree-Fock approach to the perturbation-theoretic study of many-fermion systems arises from the possible singular nature of the two-body force as appears, e.g., in He^3 atoms and nucleons. The Brueckner-Hartree-Fock and the Bethe-Brandow-Petschek theories (both of which retain the idea of real single-particle energies, orbital eigenfunctions

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and a hermitean common potential) are deduced from the diagrammatic Dyson equation for the exact one-particle Green function, Consequently, the set of assumptions that must go into this equation in order to obtain the different variants of Brueckner theory are rendered transparent and compact.

1. ORDINARY FORMULATION OF HARTREE-FOCK THEORY

There exist several formulations[1] of the Hartree-Fock approximation; we review briefly that of Goldstone which has been useful for previous discussions of Brueckner theory. Consider an N-nucleon system with hamiltonian

$$H = T + v \tag{1a}$$

where

$$T \equiv -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 \quad \text{and} \quad v \equiv \sum_{i<j}^{N} v_{ij} \tag{1b}$$

and consider also the reconstruction

$$H = H_0 + V \tag{2a}$$

with

$$H_0 \equiv \sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla_i^2 + U_i\right) \text{ and } V \equiv \sum_{i<j}^{N} v_{ij} - \sum_{i=1}^{N} U_i \tag{2b}$$

where U_i is an as yet undetermined single-particle operator, the choice of which will control the convergence rate of a subsequent perturbation expansion in terms of the residual interaction V with the eigenstates of the unperturbed hamiltonian H_0 as a basis. Requirement that the expectation value of H calculated between the lowest energy eigenstate of H_0 be stationary gives the HF choice of H_0 and leads to a set of N coupled, one-particle, Schroedinger-like non-linear equations with a non-local potential well:

$$-\frac{\hbar^2}{2m}\nabla_1^2\,\varphi_i(\boldsymbol{x}_1)+U_1\,\varphi_i(\boldsymbol{x}_1)=\epsilon_i\,\varphi_i(\boldsymbol{x}_1) \tag{3a}$$

$$U_1\,\varphi_i(\boldsymbol{x}_1)\equiv\int d\boldsymbol{x}_2\,v(|\boldsymbol{x}_1-\boldsymbol{x}_2|)\sum_{j=1}^{N}\{\varphi_j^*(\boldsymbol{x}_2)\,\varphi_j(\boldsymbol{x}_2)\,\varphi_i(\boldsymbol{x}_1)-$$

$$-\varphi_j^*(\boldsymbol{x}_2)\,\varphi_j(\boldsymbol{x}_1)\,\varphi_i(\boldsymbol{x}_2)\} \tag{3b}$$

$$\int d\boldsymbol{x}\,\varphi_i(\boldsymbol{x})\,\varphi_j(\boldsymbol{x})=\delta_{ij} \tag{3c}$$

where $\int d\boldsymbol{x}$ means integration over continuous and summation over discrete variables. In occupation-number representation Eqs. (2) become

$$H_0=\sum_i \epsilon_i\,a_i^+ a_i \tag{4a}$$

$$V=\frac{1}{2}\sum_{ijkl} v_{ij,kl}^{\mathrm{HF}}\,a_i^+ a_j^+ a_l\,a_k-\sum_{ij} U_{ij}^{\mathrm{HF}}\,a_i^+ a_j \tag{4b}$$

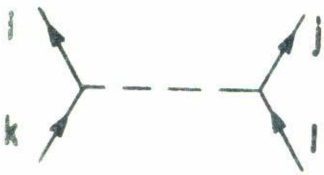
$$v_{ij,kl}^{\mathrm{HF}}\equiv\int d\boldsymbol{x}_1\int d\boldsymbol{x}_2\,\varphi_i^*(\boldsymbol{x}_1)\,\varphi_j^*(\boldsymbol{x}_2)\,v(|\boldsymbol{x}_1-\boldsymbol{x}_2|)\,\varphi_k(\boldsymbol{x}_1)\,\varphi_l(\boldsymbol{x}_2) \tag{5}$$

$$U_{ij}^{\mathrm{HF}}\equiv\int d\boldsymbol{x}_1\,\varphi_i^*(\boldsymbol{x}_1)\,U_1\,\varphi_j(\boldsymbol{x}_1) \tag{6}$$

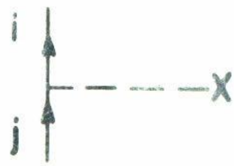
and the label HF is introduced to stress the fact that Eqs. (5) and (6) are calculated with the HF solutions of Eqs. (3). If the lowest eigenvalue of Eq. (4) is *non-degenerate* then the total ground-state energy of the system is[2]

$$E=W_0+\delta E=\sum \epsilon_i\,n_i+\delta E \tag{7}$$

where the first term on the r.h.s. is the lowest eigenvalue of H_0, i.e., the state with $n_i=1$ for the lowest N single-particle states and $n_i=0$ for the rest, and the energy shift δE is expressible as a sum of contributions from all corresponding Feynman diagrams. These diagrams possess two kinds of vertices: a) the four-vertices and b) the pair-vertices



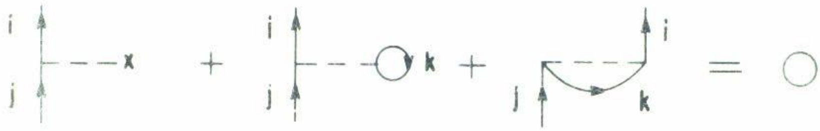
$-\frac{i}{\hbar} v^{\mathrm{HF}}_{ij,kl}$;



$+\frac{i}{\hbar} U^{\mathrm{HF}}_{ij}$

(8)

shown with their respective contributions. The HF choice of U is such that always the sum of the three fragments



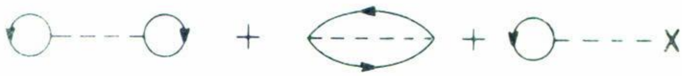
(9)

is cancelled exactly. In view of Eq. (8), and the rule that a hole line (occupied orbit) as well as a closed-fermion loop each give a minus sign, just means that

$$U^{\mathrm{HF}}_{ij} = \sum_k \tilde{v}^{\mathrm{HF}}_{ik,jk} n_k , \tag{10a}$$

$$\tilde{v}_{ij,kl} \equiv v_{ij,kl} - v_{ij,lk} . \tag{10b}$$

The HF energy shift δE^{HF} is obtained by restricting the infinite set of diagrams determining δE in Eq. (7) to all *first order* vacuum diagrams, namely

$\delta E =$ 

(11)

so that Eq. (8) and the abovementioned rule, as well as the additional new rule that to each vacuum diagram one ascribes the factor $i\hbar/g$, where $g = 2$ or 1 according as the diagram has or does not have left-right symmetry, gives

$$\delta E^{\mathrm{HF}} = \frac{1}{2} \sum_{ij} \tilde{v}^{\mathrm{HF}}_{ij,ij} n_i n_j - \sum_i U^{\mathrm{HF}}_{ii} n_i \tag{12}$$

This together with Eqs. (7) and (10) finally gives

$$\begin{aligned} E^{\mathrm{HF}} &= \sum_i \epsilon_i n_i - \frac{1}{2} \sum_{ij} \tilde{v}^{\mathrm{HF}}_{ij,ij} n_i n_j \\ &= \sum_i \left(\epsilon_i - \frac{1}{2} U^{\mathrm{HF}}_{ii} \right) n_i \end{aligned} \tag{13}$$

whereby it is clear that, in this approximation, the original system of interacting ***bare*** particles has been replaced by one of non-interacting ***dressed*** (or ***quasi***) particles which are completely defined by the set of single-particle (real) energies and orbital states $\{ \epsilon_i , \varphi_i(x_1) \mid i = 1, 2, \ldots N; N+1, \ldots \infty \}$ or, equivalently, by the specification of the self-consistent field operator U_1.

This very simple and physically appealing formalism must however, be abandoned in any reasonable generalization of the HF approximation. Nevertheless, it is convenient to preserve the main point of the above picture: the replacement of an interacting system of bare particles by some ideal system of non-interacting dressed particles, ***except*** that now one must allow for the possibility that the new quasiparticles might possess non-infinite lifetimes. In that event, it will be impossible, in principle, to characterize these quasi-particles with ***real*** energies ϵ_i and three-dimensional spatial functions $\varphi_i(x_1)$ which describe only ***stationary*** states. By the same token, the concept of a hermitean potential field operator U_1 will no longer be useful. On the other hand, the *one-particle Green function*, or propagator, avoids these notions and is indeed found useful for a generalization of HF theory. We thus introduce it below by formulating ordinary HF theory.

2. ONE-PARTICLE GREEN FUNCTION FORMULATION

Before defining the one-particle Green function consider the orthonormal set of (plane-wave) solutions of the zero-order hamiltonian of Eq. (1); for particle 1 we have

$$-\frac{\hbar^2}{2m}\nabla_1^2\, \psi_i(x_1) = T_i\, \psi_i(x_1)\ ;$$

where

$$T_i \equiv \hbar^2 k_i^2/2m\ ,$$

and

$$\psi_i(x_1) = \Omega^{-\frac{1}{2}} e^{ik_i \cdot r_1}\, \delta_{s_i,\sigma_1}\, \delta_{t_i,\tau_1}$$

with

$$\int dx_1\, \psi_i^*(x_1)\, \psi_j(x_1) = \delta_{ij} \tag{14}$$

with Ω the normalization volume. In occupation-number representation this gives

$$H = T + v$$

with

$$T = \sum_i T_i\, a_i^+ a_i\ ;\ v = \frac{1}{2} \sum_{ijkl} v_{ij,kl}\, a_i^+ a_j^+ a_l a_k \tag{15a}$$

and

$$v_{ij,kl} \equiv \int dx_1 \int dx_2 \psi_i^*(x_1)\, \psi_j^*(x_2)\, v(x_1 - x_2)\, \psi_k(x_1)\, \psi_l(x_2)\,. \quad (15b)$$

The eigenfunctions defined by Eq. (14), as well as those of the HF Eqs. (3), form a complete, orthonormal set related by the unitary transformation

$$\varphi_i(x) = \sum_j c_{ji}\, \psi_i(x)\,;\;\; \psi_i(x) = \sum_i c_{ji}^*\, \varphi_i(x) \quad (16a, b)$$

$$\sum_k c_{ik}^* c_{jk} = \delta_{ij} = \sum_k c_{ki}^* c_{kj}\,. \quad (16c)$$

Since the fermi operators α_i^+, α_i create and annihilate particles in the HF state $\varphi_i(x)$, while a_i^+, a_i do so in the free state $\psi_i(x)$, Eqs. (16) lead to the canonical transformations

$$\alpha_i = \sum_j c_{ji}^* a_j\,;\;\; a_j = \sum_i c_{ji}\, \alpha_i\,. \quad (17a, b)$$

Then the field and number operators, respectively, can be written

$$\psi(x) = \sum_j \varphi_i(x)\, \alpha_j = \sum_i \psi_i(x)\, a_i \quad (18)$$

$$n = \sum_j \alpha_j^+ \alpha_j = \sum_i a_i^+ a_i \quad (19)$$

Finally, because of Eq. (16a) we note that Eqs. (5) and (15b) are related by

$$v_{ij,kl}^{\mathrm{HF}} = \sum_{mnpq} c_{mi}^* c_{nj}^* c_{pk} c_{ql} v_{mn,pq}\,. \quad (20)$$

Again, assuming the lowest eigenvalue of the unperturbed hamiltonian T to be non-degenerate, the ground-state energy of H will now be

$$E = E_0 + \Delta E = \sum_i T_i n_i + \Delta E \quad (21)$$

with ΔE the energy-shift based on the free-particle unperturbed hamiltonian T.

The one-particle Green function is defined as

$$G_{ij}(t-t') \equiv \langle T\{a_i(t)\, a_j^+(t')\}\rangle$$

$$\equiv \langle a_i(t)\, a_j^+(t')\,\theta(t-t') - a_j^+(t')\, a_i(t)\,\theta(t'-t)\rangle$$

$$\equiv \theta(t-t')\,\tilde{\tilde{G}}_{ij}(t-t') + \theta(t'-t)\,\tilde{G}_{ij}(t-t') \qquad (22)$$

with

$$a_i(t) \equiv \exp\left[\frac{i}{\hbar}Ht\right] a_i \exp\left[-\frac{i}{\hbar}Ht\right] \qquad (22a)$$

where expectation values are taken between exact, fully interacting, ground-state eigenfunctions of H. The ***bare*** one-particle propagator is now obtained from Eq. (22) by replacing everywhere in it H by the pure kinetic energy operator T, since then $a_i(t) = \exp\left[-\frac{i}{\hbar}T_i t\right] a_i$ from Eq. (22a), so that

$$G^0_{ij}(\tau) \equiv \delta_{ij}\, G^0_i(\tau)$$

$$G^0_i(\tau) \equiv \exp\left[-\frac{i}{\hbar}T_i\tau\right]\{(1-n_i)\,\theta(\tau) - n_i\,\theta(-\tau)\}. \qquad (23)$$

Also, using Eq. (17b) in Eq. (22) with H replaced by H_0, and noting that $\alpha_j(t) = \exp\left[-\frac{i}{\hbar}\epsilon_j t\right]\alpha_j$, one gets the HF ***dressed*** one-particle propagator.

$$G^{\mathrm{HF}}_{ij}(\tau) = \sum_k c_{ik}\, c^*_{jk} \exp\left[-\frac{i}{\hbar}\epsilon_k\tau\right]\{(1-n_k)\,\theta(\tau) - n_k\,\theta(-\tau)\}$$

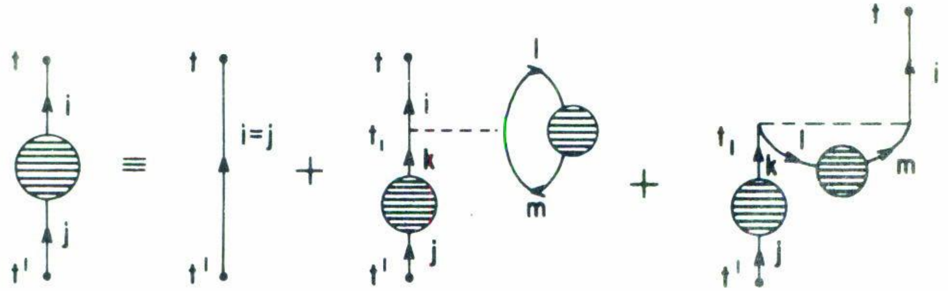
$$\equiv \theta(\tau)\,\tilde{\tilde{G}}^{\mathrm{HF}}_{ij}(\tau) + \theta(-\tau)\,\tilde{G}^{\mathrm{HF}}_{ij}(\tau). \qquad (24)$$

Knowledge of the exact (or approximate) diagonal ***retarded*** one-particle Green function $\tilde{G}_{jj}(\tau)$ in Eq. (22) is sufficient to determine the exact (or approximate) energy shift of Eq. (21), since (see Appendix)

$$\Delta E = \frac{1}{2}\int_0^1 \frac{dg}{g} \sum_j \left[\left(\frac{\hbar}{i}\frac{\partial}{\partial t} + T_j\right) \tilde{G}_{jj}(t, t'|g)\right]_{t'=t} \tag{25}$$

where g is the coupling constant in $H(g) = T + gv$. This formula allows the calculation of approximate values of ΔE, and hence of E by Eq. (21), *solely* on the basis of the corresponding approximate form of $\tilde{G}_{jj}(t, t'|g)$.

The HF-***dressed*** propagator is ***defined*** diagrammatically by



(26)

and formally by

$$G_{ij}^{\mathrm{HF}}(t-t') \equiv G_i^0(t-t')\,\delta_{ij} + $$

$$+\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt_1 \sum_{klm} \tilde{v}_{il,km}\, G_i^0(t-t_1)\, G_{ml}^{\mathrm{HF}}(-0)\, G_{kj}^{\mathrm{HF}}(t_1-t') \tag{27}$$

where Eq. (10b) has been used to express both direct and exchange contributions in a single term. Combining this with Eqs. (23) and (24), integrating over times (after introducing the proper convergence factors) and using the unitarity relations Eqs. (16c), one obtains

$$(T_i - \epsilon_j)\, c_{ij} + \sum_{klm} \tilde{v}_{il,km} \left(\sum_s c_{ms} c^*_{ls} n_s\right) c_{kj} = 0\,. \qquad (28)$$

This infinite set of coupled algebraic equations obviously contains the same information as the ordinary HF equations (3) for both occupied (here $n_i = 1$) as well as unoccupied (here $n_i = 0$) states.

It must be verified that this new formulation of HF theory is indeed equivalent to other forms, in particular to that of Section I. Let us calculate the integrand in Eq. (25) with the retarded part of the HF-*dressed* propagator of Eq. (24); one has

$$\frac{1}{2}\sum_j \left(\frac{\hbar}{i}\frac{\partial}{\partial t} + T_j\right) G^{\mathrm{HF}}_{jj}(t, t'|g)\Bigg|_{t'=t} = \frac{1}{2}\sum_{ij}(\epsilon_j - T_i)\, c_{ij} c^*_{ij} n_j =$$

$$= \frac{g}{2}\sum_{ilkm} \tilde{v}_{il,km}\left(\sum_s c_{ms} c^*_{ls} n_s\right)\left(\sum_j c_{kj} c^*_{ij} n_j\right), \qquad (29)$$

the last step following from Eq. (28) with $v \to gv$. Now Eq. (20) for $v \to gv$ in Eq. (13) gives

$$E^{\mathrm{HF}}(g) = \sum_i \epsilon_i n_i - \frac{g}{2}\sum_{mnpq} \tilde{v}_{mn,pq}\left(\sum_s c^*_{ms} c_{ps} n_s\right)\left(\sum_j c^*_{nj} c_{qj} n_j\right) \qquad (30)$$

from which, upon noting that both ϵ's and c's now depend on g, we have

$$\frac{dE^{\mathrm{HF}}(g)}{dg} = \sum_i \frac{d\epsilon_i}{dg} n_i - \frac{1}{2}\sum_{mnpq} \tilde{v}_{mn,pq}\left(\sum_s c^*_{ms} c_{ps} n_s\right)\left(\sum_j c^*_{nj} c_{qj} n_j\right) -$$

$$- g\sum_{mnpq} \tilde{v}_{mn,pq}\left(\sum_j c^*_{nj} c_{qj} n_j\right)\left[\sum_s \left\{\frac{dc^*_{ms}}{dg} c_{ps} + c^*_{ms}\frac{dc_{ps}}{dg}\right\} n_s\right]. \qquad (31)$$

On the other hand, Eq. (28) for $H(g) = T + gv$, after deriving with respect to g, multiplying by $c^*_{ij} n_j$, summing over (i, j) and again using Eq. (28), gives

$$-\sum_j \frac{d\epsilon_j}{dg} n_j + \sum_{ilkm} \tilde{v}_{il,km} \left(\sum_r c_{mr} c^*_{lr} n_r \right)\left(\sum_s c_{ks} c^*_{is} n_s \right) +$$

$$+ g \sum_{ilkm} \tilde{v}_{il,km} \left(\sum_s c_{ks} c^*_{is} n_s \right) \left[\sum_r \left\{ c_{mr} \frac{dc^*_{lr}}{dg} + \frac{dc_{mr}}{dg} c_{lr} \right\} n_r \right] = 0 . \tag{32}$$

This equation permits eliminating all derivative terms in r.h.s. of Eq. (31) leaving, since $d/dg\, \Delta E(g) = d/dg\, [E(g) - E_0] = dE(g)/dg$, the result

$$\frac{d\Delta E^{\mathrm{HF}}(g)}{dg} = \frac{1}{2} \sum_{ijkl} \tilde{v}_{ij,kl} \left(\sum_s c^*_{is} c_{ks} n_s \right)\left(\sum c^*_{jr} c_{lr} n_r \right) . \tag{33}$$

Finally, comparison of Eqs. (33) and (29) leads to

$$g\, \frac{d\Delta E^{\mathrm{HF}}(g)}{dg} = \frac{1}{2} \sum_j \left[\left(\frac{\hbar}{i} \frac{\partial}{\partial t} + T_j \right) \tilde{G}^{\mathrm{HF}}_{jj}(t, t' | g) \right]_{t'=t} \tag{34}$$

or, since $\Delta E^{\mathrm{HF}}(0) = 0$,

$$\Delta E^{\mathrm{HF}} = \frac{1}{2} \int_0^1 \frac{dg}{g} \sum_j \left[\left(\frac{\hbar}{i} \frac{\partial}{\partial t} + T_j \right) \tilde{G}^{\mathrm{HF}}_{jj}(t, t' | g) \right]_{t'=t} . \tag{35}$$

To summarize, the result just obtained for ΔE^{HF} follows basically from Eqs. (13), (23), (24) and (27).

To complete the proof of equivalence between the two formulations of HF theory thus far presented, we must show that the HF equations (28) can indeed be obtained from Eqs. (3), (9) and (10). Using Eq. (16) one can transform Eq. (3a) into

$$(T_j - \epsilon_i)\, c_{ji} + \sum_k c_{ki} U_{jk} = 0 . \tag{36}$$

Again, if Eq. (16) is used in Eqs. (10) together with (20), one gets

$$\sum_{pq} c^*_{pi} c_{qj} U_{pq} = \sum_k n_k \sum_{mnpq} c^*_{mi} c^*_{nk} c_{pj} c_{qk} \tilde{v}_{mn,pq} . \qquad (37)$$

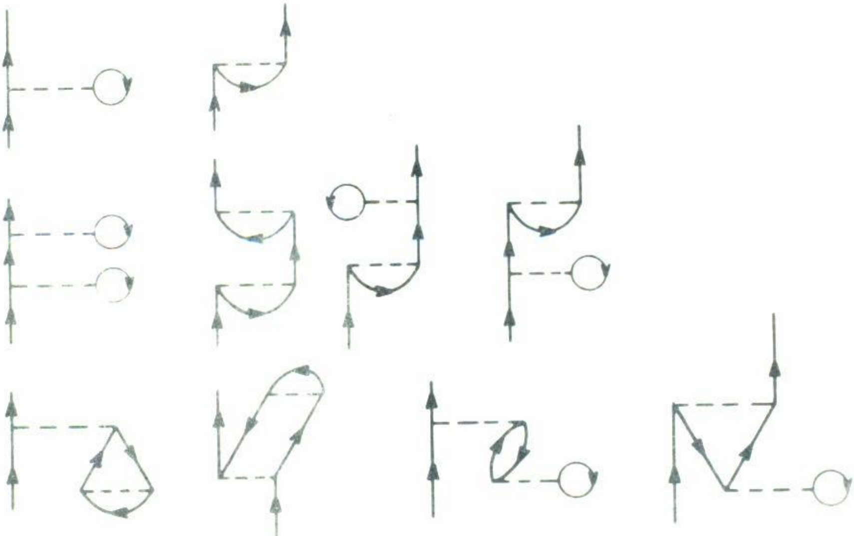
Use of Eq. (16c) reduces this to

$$U_{jk} = \sum_{mq} \tilde{v}_{jm,kq} \Big(\sum_s c^*_{ms} c_{qs} n_s \Big) \qquad (38)$$

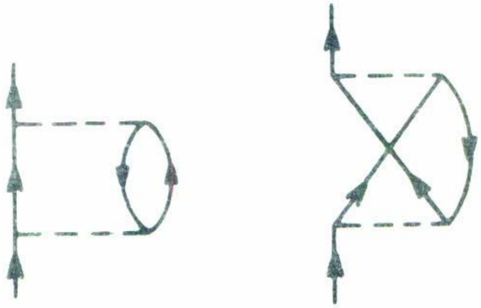
which when inserted into Eq. (36) gives just Eq. (28).

Note that from the basic definition Eq. (26) of the HF-dressed one-particle propagator, the free one-particle propagator is being dressed *only* with the so-called *first-order* self-energy parts, namely

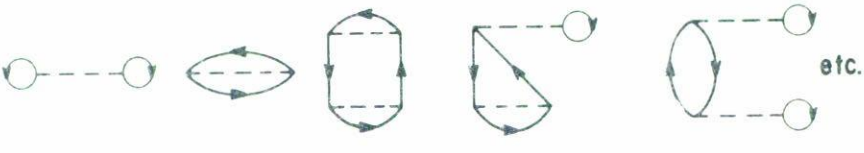
but account is taken of the possibility of inserting these parts into one another an arbitrary number of times up to infinity. Thus, in first and second orders one includes into G^{HF}_{ij} the following diagrams:



but *not* the diagrams:



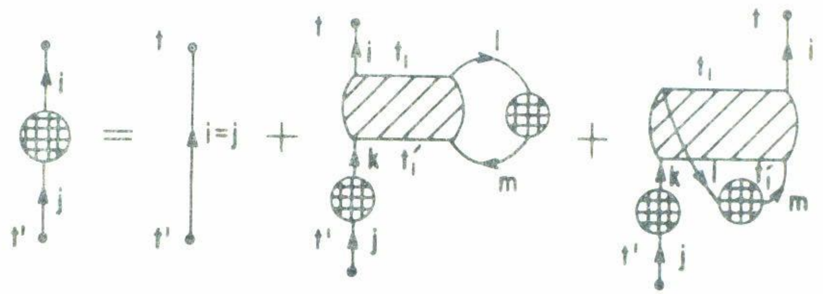
which are ***second***-order self-energy parts. Correspondingly in ΔE^{HF} one is incorporating contributions of *vacuum* diagrams which are contracted from the first-order self-energy parts mentioned above, i. e., whose external lines are joined together. So, in first and second orders, for example, one includes into ΔE^{HF} the diagrams



but *not* the diagrams

3. GENERALIZED BRUECKNER-HARTREE-FOCK THEORY

Consider the generalization of the HF theory developed above, consisting in defining a new one-particle propagator $G_{ij}^{\mathrm{BHF}}(t-t')$ as



(39)

or, formally as

$$G_{ij}^{\mathrm{BHF}}(t-t') = G_{ij}^{0}(t-t')\,\delta_{ij} +$$

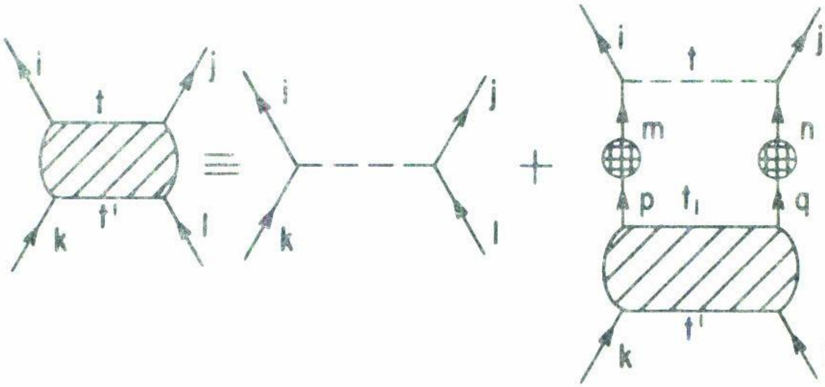
$$+\frac{i}{\hbar}\int_{-\infty}^{+\infty}dt_1\int_{-\infty}^{+\infty}dt_1'\sum_{klm}\tilde{K}_{il,km}(t_1-t_1')\,G_i^0(t-t_1)\,G_{ml}^{\mathrm{BHF}}(t_1'-t_1-0)\,G_{kj}^{\mathrm{BHF}}(t_1'-t'),$$

(39a)

with

$$\tilde{K}_{il,km}(\tau) \equiv K_{il,km}(\tau) - K_{il,mk}(\tau).$$

The shaded "blob" in Eq. (39) is a generalized Brueckner reaction matrix defined as $-\frac{i}{\hbar}K_{ij,kl}(t-t')$ or



(40a)

and formally as

$$K_{ij,kl}(t-t') = v_{ij,kl}\,\delta(t-t') -$$

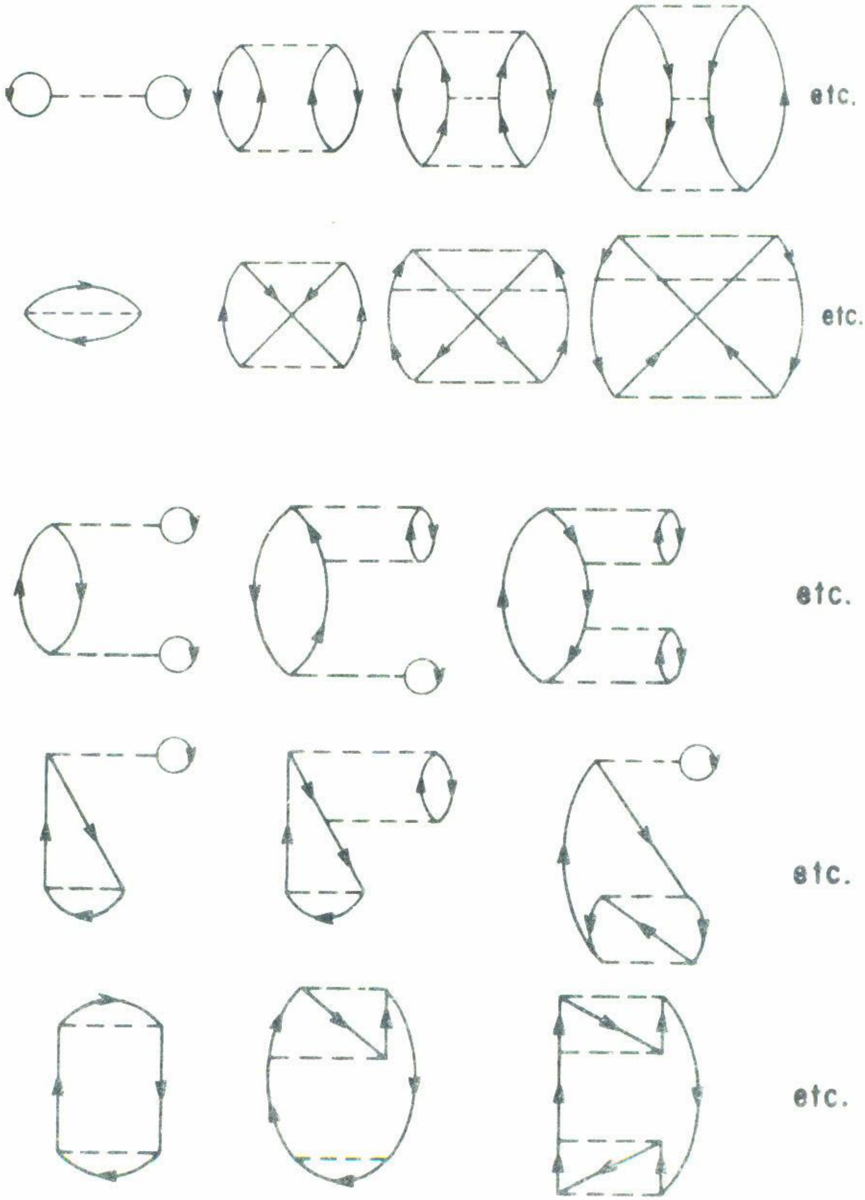
$$-\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt_1 \sum_{pqmn} v_{ij,mn}\, G^{\mathrm{BHF}}_{mp}(t-t_1)\, G^{\mathrm{BHF}}_{nq}(t-t_1)\, K_{pq,kl}(t_1-t') \,. \quad (40b)$$

The above formulation is *more general* than the usual BHF theory in that *both* particle-particle as well as hole-hole ladders[3] are included, since in Eqs. (40) $t > t_1$ as well as $t < t_1$ are possible. Also, as is clear from Eqs. (39), ladder insertions are possible *both* in hole as well as particle lines. The *vacuum* diagrams whose contributions are accounted for in

$$\Delta E^{\mathrm{BHF}} = \frac{1}{2}\int_0^1 \frac{dg}{g} \sum_j \left[\left(\frac{\hbar}{i}\frac{\partial t}{\partial} + T_j\right) G^{\mathrm{BHF}}_{jj}(t,t'\,|\,g)\right]_{t'=t} \quad (41)$$

are analogous to those included in calculating ΔE^{HF} previously, except that instead of the "bare" v-interaction lines we now have K-interaction "blobs".

For example, into ΔE^{BHF} one incorporates the following diagrams



Note that *all* first-and second-order vacuum diagrams are included in ΔE^{BHF}. Also, many but not all third order diagrams are included; in particular one is including third-order diagrams with self-energy insertions of the first *and* second order but one is not including third order diagrams like

etc.

Now, it seems that in principle it is impossible to reformulate the above *generalized* BHF theory in such a way that the notion of real single-particle energies, orbital eigenfunctions and hermitean common potential-well is retained. Nonetheless it is possible to introduce certain approximations which allows us to keep this picture and we now examine this in detail obtaining the usual Brueckner-Hartree-Fock[7] as well as the Bethe-Brandow and Petschek[8] schemes.

Consider the effective interaction K-operator in Eqs. (39) to act *instantaneously* namely put

$$\tilde{K}_{ij,km}(t_1 - t_1') = \delta(t_1 - t_1')\,\tilde{K}^{\mathrm{BHF}}_{ij,km} \; . \qquad (42)$$

This assumption makes Eq. (39a) entirely analogous to Eq. (27) of ordinary HF theory so that, correspondingly, one now has, instead of Eq. (24), putting $\hbar = 1$,

$$G^{\mathrm{BHF}}_{ij}(t-t') = \sum_k c_{ik}c^*_{jk}\exp\left[-i\epsilon_k(t-t')\right]\left\{(1-n_k)\,\theta(t-t') - n_k\,\theta(t'-t)\right\}$$

$$= \theta(t-t')\,\tilde{\tilde{G}}^{\mathrm{BHF}}_{ij}(t-t') + \theta(t'-t)\,\tilde{G}^{\mathrm{BHF}}_{ij}(t-t') \qquad (43)$$

where the c's and ϵ's of this expression now satisfy the BHF equations

$$(T_i - \epsilon_j)\,c_{ij} + \sum_{klm}\tilde{K}^{\mathrm{BHF}}_{il,km}\left(\sum_s c_{ms}c^*_{ls}n_s\right)c_{kj} = 0 \qquad (44)$$

which are formally the same as the HF equations (28) except that the bare interaction operator v is replaced by the (instantaneous) reaction operator K^{BHF}.

Moreover, as in obtaining Eq. (30) previously, one now gets

$$E^{\mathrm{BHF}} = \sum_i \epsilon_i n_i - \frac{1}{2} \sum_{mnpq} \tilde{K}^{\mathrm{BHF}}_{mn,pq} \Big(\sum_r c^*_{mr} c_{pr} n_r\Big)\Big(\sum_s c^*_{ns} c_{qs} n_s\Big)$$

$$= \sum_i \Big(\epsilon_i - \frac{1}{2} \mathcal{U}_i^{\mathrm{BHF}}\Big) n_i \tag{45}$$

where we have defined

$$\mathcal{U}_i^{\mathrm{BHF}} \equiv \sum_{jk} U^{\mathrm{BHF}}_{jk} c^*_{ji} c_{ki} \,, \tag{46}$$

$$U^{\mathrm{BHF}}_{jk} \equiv \sum_{lm} \tilde{K}^{\mathrm{BHF}}_{jl,km} \Big(\sum_s c^*_{ls} c_{ms} n_s\Big) \,. \tag{47}$$

Equations (44) to (47) constitute the basic expressions of standard BHF theory. Now the main assumption Eq. (42) is strictly speaking not consistent with the defining Eq. (40b) for the reaction operator K. To see this, substitute Eq. (43) into Eq. (40b) and, defining

$$K_{ij,kl}(\omega) \equiv \int_{-\infty}^{+\infty} dt \exp\,[i\omega t]\, K_{ij,kl}(t) \,, \tag{48}$$

multiply the result by $\exp\,[i\omega t]$ integrating over t from $-\infty$ to $+\infty$ and making the appropriate change of variables, one obtains (with η a small positive quantity).

$$K_{ij,kl}(\omega) = v_{ij,kl} - \sum_{mnpq} v_{ij,mn} \sum_{sr} c_{ms} c^*_{ps} c_{nr} c^*_{qr}$$

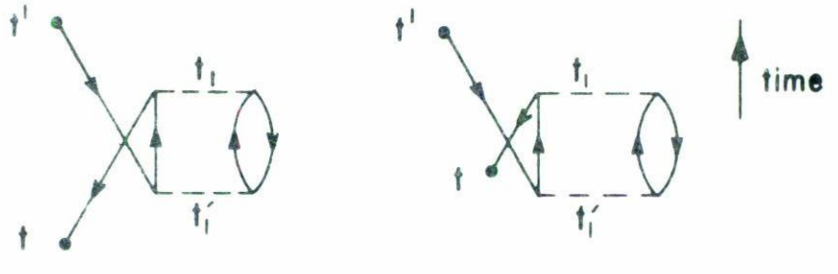
$$\left\{ \frac{(1-n_s)(1-n_r)}{\epsilon_s + \epsilon_r - \omega + i\eta} - \frac{n_r n_s}{\epsilon_s + \epsilon_r - \omega - i\eta} \right\} K_{pq,kl}(\omega) \tag{49}$$

which is clearly *inconsistent* with Eqs. (42) and (48) which would give

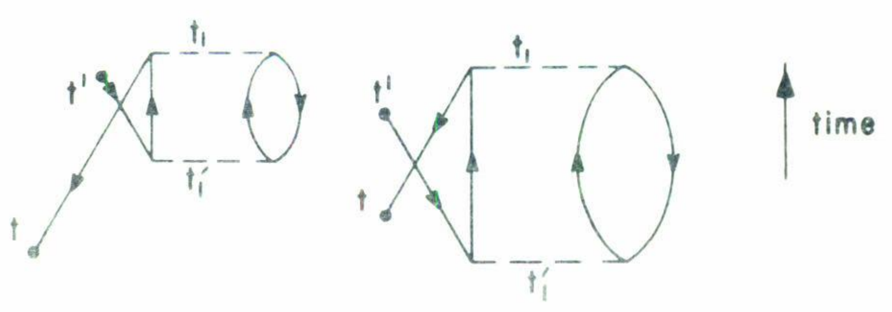
$$K_{ij,kl}(\omega) = K^{\rm BHF}_{ij,kl} \quad , \tag{50}$$

i.e., energy-independence of the reaction operator. Standard BHF theory *ignores the last term*[5,6] in Eq. (49) and furthermore attempts to reconcile Eqs. (49) and (50) by using an "average" value of ω.

Finally, we discuss the Bethe-Brandow-Petschek theorem,[8] which is essentially a scheme that again permits a standard single-particle interpretation of Brueckner theory. The assumptions applied to the general formalism Eqs. (39) to (40) are: a) neglect completely all hole-hole ladders in Eqs. (40), b) replace all *particle* propagators by their zero-order approximation Eq. (23) and c) in dressing the bare *hole* lines consider only a certain class of insertions namely, those with time-orderings like, e.g., for second-order insertions:



– but *neglect* those insertions with time orders like



Put briefly, in the BBP theory only hole lines appear dressed and then only with a restricted class of particle-particle ladders. The reason for assumption (c) is just summability of the selected set of insertions. Hence in the BBP theory instead of Eq. (39a) one has: for $t < t'$ (hole propagator)

$$G_{ij}^{\mathrm{BBP}}(t-t') = G_i^0(t-t')\,\delta_{ij} + \frac{i}{\hbar}\int_t^{t'} dt_1 \int_{-\infty}^{t_1} dt_1' \sum_{klm} \tilde{K}_{il,km}^{\mathrm{BBP}}(t_1 - t_1')$$

$$\times G_i^0(t-t_1)\, G_{ml}^{\mathrm{BBP}}(t_1'-t_1-0)\, G_{kj}^{\mathrm{BBP}}(t_1'-t') \tag{51a}$$

and for $t > t'$ (particle propagator) just

$$G_{ij}^{\mathrm{BBP}}(t-t') = G_i^0(t-t')\,\delta_{ij}\,. \tag{51b}$$

Instead of Eq. (40b) one now has for the BBP reaction operator: for $t < t'$,

$$K_{ij,kl}^{\mathrm{BBP}}(t-t') = 0 \tag{52a}$$

while, for $t > t'$,

$$K_{ij,kl}^{\mathrm{BBP}}(t-t') = v_{ij,kl}\,\delta(t-t'-0) - \frac{i}{\hbar}\int_{t'}^{t} dt_1 \sum_{pq} v_{ij,pq}\, G_p^0(t-t_1)$$

$$\times G_q^0(t-t_1)\, K_{pq,kl}^{\mathrm{BBP}}(t-t_1) \tag{52b}$$

and we note that K^{BBP} is defined less restrictively than K^{BHF} above, Eq. (42). Combining these two equations with Eq. (23) one obtains, for τ positive only of course,

$$K_{ij,kl}^{\mathrm{BBP}}(\tau) = v_{ij,kl}\,\delta(\tau-0) - \frac{i}{\hbar}\int_{-\infty}^{\tau} dt_1 \sum_{pq} v_{ij,pq}(1-n_p)(1-n_q)\,\cdot$$

$$\cdot\,\exp\left[-\frac{i}{\hbar}(T_p + T_q)(\tau - t_1)\right] K_{pq,kl}^{\mathrm{BBP}}(t_1) \tag{53}$$

whose Fourier transform by Eq. (48) is

$$K^{\mathrm{BBP}}_{ij,kl}(\omega) = v_{ij,kl} - \sum_{pq} v_{ij,pq} \frac{(1-n_p)(1-n_q)}{T_p + T_q - \omega} K^{\mathrm{BBP}}_{pq,kl}(\omega) \tag{54}$$

Equations (51) can now be solved by writing, in analogy with Eq. (24) for the ordinary HF-dressed propagator,

$$G^{\mathrm{BBP}}_{ij}(t-t') = \exp\left[-\frac{i}{\hbar} T_i (t-t')\right](1-n_i)\, \delta_{ij}\, \theta(t-t') -$$

$$- \sum_s c_{is} c^*_{js} n_s \exp\left[-\frac{i}{\hbar} \epsilon_s (t-t')\right] \theta(t'-t) \tag{55}$$

$$\equiv \theta(t-t')\, \tilde{\tilde{G}}^{\mathrm{BBP}}_{ij}(t-t') + \theta(t'-t)\, \tilde{G}^{\mathrm{BBP}}_{ij}(t-T'),$$

the first term on the r.h.s. being the particle- and the second term the hole-propagator and where the c's and ϵ's are yet to be determined. Combining Eqs. (55) and (23) into Eq. (51a), using Eq. (16c) and Eq. (48), one arrives at

$$(T_i - \epsilon_s)\left(n_i \exp\left[-\frac{i}{\hbar} T_i t\right] - n_s \exp\left[-\frac{i}{\hbar} \epsilon_s t\right]\right) c_{is} +$$

$$+ \sum_{klm} \sum_r \tilde{K}^{\mathrm{BBP}}_{il,km}(\epsilon_r + \epsilon_s)\, c_{mr} c^*_{lr} n_r c_{ks} \left(\exp\left[-\frac{i}{\hbar} T_i t\right] - \exp\left[-\frac{i}{\hbar} \epsilon_s t\right]\right) n_i n_s = 0\,.$$

Thus, it follows directly that for occupied states s and i, $n_s = n_i = 1$:

$$(T_i - \epsilon_s)\, c_{is} + \sum_{klm} \sum_r \tilde{K}^{\mathrm{BBP}}_{il,km}(\epsilon_r + \epsilon_s)\, c_{mr} c^*_{lr} n_r c_{ks} = 0 \tag{57a}$$

while for unoccupied states s and i, $n_s = n_i = 0$:

$$c_{is} = \delta_{is}\,, \quad \epsilon_i = T_i \tag{57b}$$

and for s and i such that either $n_s = 0$, $n_i = 1$ or $n_s = 1$, $n_i = 0$:

$$c_{is} = 0 \,. \tag{57c}$$

Finally, Eqs. (55) to (57) used in the equation

$$\Delta E^{\mathrm{BBP}} \leq \frac{1}{2}\int_0^1 \frac{dg}{g} \sum_j \left[\left(\frac{\hbar}{i}\frac{\partial}{\partial t} - T_j\right)\tilde{G}_{ij}^{\mathrm{BBP}}(t,t'\,|\,g)\right]_{t'=t} \tag{58}$$

gives, analogously as before,

$$E^{\mathrm{BBP}} = \sum_s \epsilon_s n_s - \frac{1}{2}\sum_{ijkl}\sum_{rs} \tilde{K}_{ij,kl}^{\mathrm{BBP}}(\epsilon_r + \epsilon_s)\, c_{is}^* c_{ks} c_{jr}^* c_{lr} n_s n_r$$

$$\equiv \sum_s \left(\epsilon_s - \frac{1}{2}\mathcal{U}_s^{\mathrm{BBP}}\right) n_s \tag{59a}$$

where one defines

$$\mathcal{U}_s^{\mathrm{BBP}} \equiv \sum_{ik} U_{ik}^{\mathrm{BBP}}(s)\, c_{is}^* c_{ks} \tag{59b}$$

$$U_{ik}^{\mathrm{BBP}}(s) \equiv \sum_{jlr} \tilde{K}_{ij,kl}^{\mathrm{BBP}}\, c_{jr}^* c_{lr} n_r \tag{59c}$$

which are the basic equations of BBP theory.

APPENDIX

For the hamiltonian $H(g) = T + gv$ we prove that $\Delta E \equiv E(1) - E(0)$, where $E(g) \equiv \langle\Psi(g)|H(g)|\Psi(g)\rangle$, is given by

$$\Delta E = \frac{1}{2}\int_0^1 \frac{dg}{g} \sum_j \left[\left(\frac{\hbar}{i}\frac{\partial}{\partial t} + T_j\right)\tilde{G}_{jj}(t, t'|g)\right]_{t'=t} . \qquad (I.1)$$

Using the definition Eq. (22) for the retarded Green function one has

$$\frac{\hbar}{i}\frac{\partial}{\partial t}\tilde{G}_{jj}(t, t'|g) = -\frac{\hbar}{i}\frac{\partial}{\partial t} \langle a_j^+(t')\, a_j(t)\rangle = -\langle a_j^+(t')[H, a_j(t)]\rangle$$

the last step following from Eq. (22a). In view of Eqs. (15a) with $v \to gv$

$$[H, a_j(t)] = -T_j a_j(t) - g \sum_{klm} v_{jk,lm}\, a_k^+(t)\, a_m(t)\, a_l(t)$$

so that

$$\frac{1}{2}\sum_j \left[\left(\frac{\hbar}{i}\frac{\partial}{\partial t} + T_j\right)\tilde{G}_{jj}(t, t'|g)\right]_{t'=t} = \frac{g}{2}\sum_{jklm} \langle a_j^+(t)\, a_k^+(t)\, a_m(t)\, a_l(t)\rangle$$

$$\equiv g \langle\Psi(g)|v|\Psi(g)\rangle . \qquad (I.2)$$

But

$$\frac{d}{dg}\Delta E(g) = \frac{d}{dg}[E_0 + \Delta E(g)] = \frac{d}{dg}\langle\Psi(g)|T + gv|\Psi(g)\rangle =$$

$$= \langle\Psi(g)|v|\Psi(g)\rangle ,$$

so one finally has

$$\Delta E = \int_0^1 d\Delta E(g) = \int_0^1 \langle\Psi(g)|v|\Psi(g)\rangle\, dg$$

which from Eq. (I.2) gives Eq. (I.1).

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RESUMEN

Los elementos básicos de la teoría de Hartree-Fock son la existencia de un operador hermitiano, que corresponde al potencial común de una sola partícula, y el espectro asociado de energías reales. La necesidad de emplear una teoría de Hartree-Fock renormalizada surge de la posible existencia de singularidades en la fuerza de dos cuerpos como sucede, por ejemplo, entre átomos de ^{3}He y nucleones.

Las teorías de Brueckner-Hartree-Fock y de Bethe-Brandow-Petschek (que retienen la idea de energías reales de una sola partícula, de orbitales y del potencial común hermitiano), se deducen de la ecuación diagramática de Dyson que debe satisfacer la función de Green de una partícula. Como consecuencia, las suposiciones que se deben hacer para llegar a las distintas variantes de la teoría de Brueckner, se expresan en forma compacta y clara.