DYNAMICAL Pair Excitations in the Electron Gas

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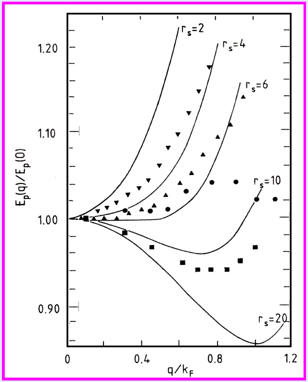
Outline

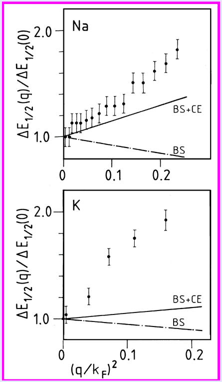
plasmons in metals

alkali metals:

EELS
experiments

vom Felde, Sprösser-Prou, Fink, PRB (89)

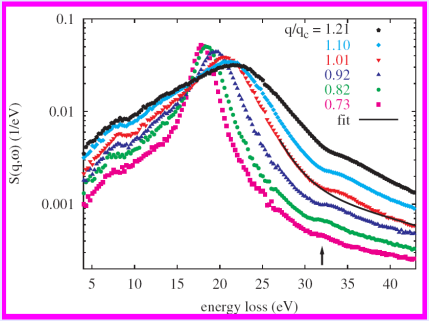


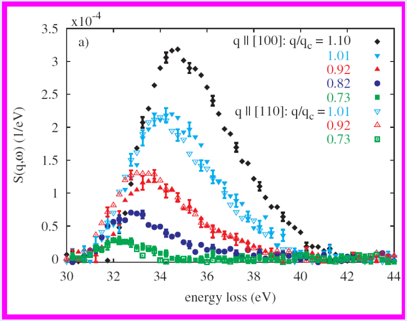


- long wavelength damping **only** explainable by multi–pair excitations
- dispersion: **both** single–pair and multi–pair correlations decrease the dispersion

recent findings

Al, Na: IXS experiments (probe larger q)





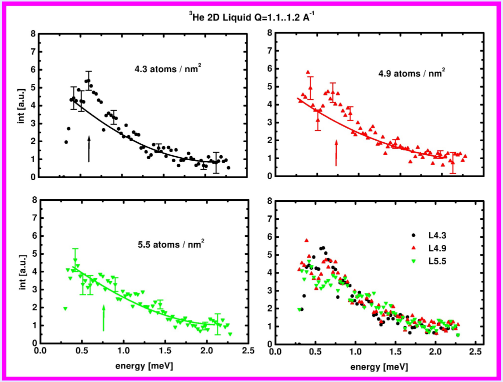
Sternemann, Huotari, Vanko, Volmer, Monaco, Gusarov, Lustfeld, Sturm, Schülke
PRL (05)

- peak clearly attributable to intrinsic **double–plasmon** excitations, genuine correlation effect, not caused by the crystal potential
- in agreement with theoretical predictions: Sturm/Gusarov, PRB (00)

dynamic structure factor of ^{3}He

$$S(q,\omega) \propto \frac{d^2\sigma}{d\omega\Omega}$$

neutron scattering experiments



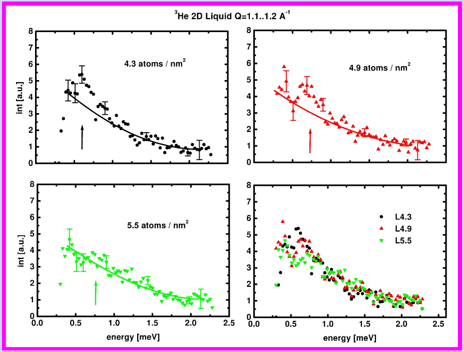
2D

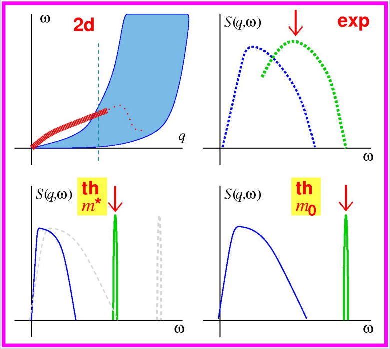
Meschke et al (2003)

- clear signature of a collective mode
- significant strength above particle–hole continuum
- energetically **much lower** than in conventional theories

m^* a possible cure ??

3D: $m_{\text{bare}} \to m^*(k) \;\Rightarrow$ theoret. collective mode adjusted to fit exp

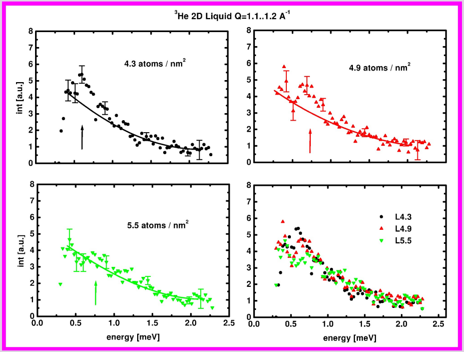


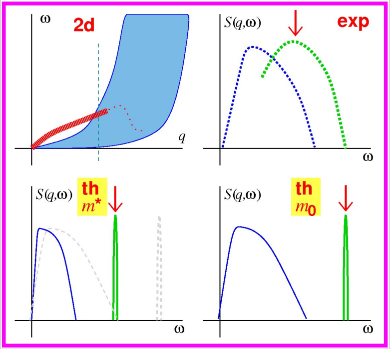


m^* a possible cure ??

3D: $m_{\mathrm{bare}} \rightarrow m^*(k) \;\Rightarrow$ theoret. collective mode adjusted to fit exp

but CANNOT shift an undamped phonon into ph–continuum





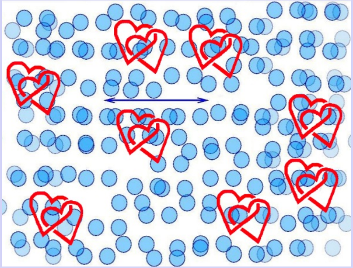
violates ω^0 & ω^1 sum rules

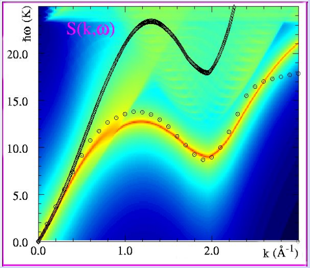
^{4} He (bosons)

- phonon-roton position needs correction when

wavelength $\lambda_{\text{phonon}} = \lambda_{\text{fluctuation}} \approx a_{\text{particles}}$ interpart. distance

- by introducing **time dependent pair correlations** $c^{(2)}$ $\widehat{=}$ backflow





Krotscheck *et al.*, LT22, (99)

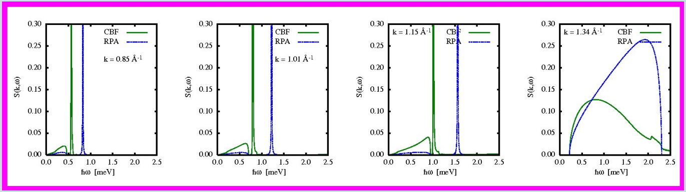
physics in ^{3}He & ^{4}He should be similar! same effects important!

We can do it BETTER than with m^*

aim(s):

- give a first–priciples description for fermions
- that invokes **dynamical** multi–particle ⟶ **pair** correlations
- and apply it to 3d & 2d ^{3}He and 3d & 2d electrons

previously reached goals



BGKLMP, CMT31, (06)

- captures the right physics, but still lacks quantitative agreement
- exp shape much broader, $q \to 0$ behavior not fully correct

Outline

1. Motivation
   - Experiments: electrons
   - Experiments: ^{3}He
   - Experiments: ^{4}He
2. Theory
   - Correlated Basis Fcts (CBF) & equs of motion (EOM)
   - response fct
   - Details
3. Results
   - Input
   - Electrons
   - Summary

Correlated Basis Fcts (CBF)

excited states

$$\psi \quad \propto \quad F \quad e^{\frac{1}{2}U} \; |\Phi_0\rangle$$

$\uparrow$ Jastrow correl. fct

$\uparrow$ Slater det

Correlated Basis Fcts (CBF)

excited states

$$\psi \;\propto\; F \; e^{\frac{1}{2}U} \; |\Phi_0\rangle$$

$\uparrow$ Jastrow correl. fct

$\uparrow$ Slater det

$$U = \sum_{ph} c^{(1)}_{ph} \, a^\dagger_p a_h + \sum_{pp'hh'} c^{(2)}_{pp'hh'} \, a^\dagger_p a^\dagger_{p'} a_h a_{h'}$$

$$\Rightarrow \quad c^{(1)} \, \Phi_{ph} \, ; \; c^{(1)} c^{(1)} \, \Phi_{php'h'} \, ; \; \ldots \, ; \quad c^{(2)} \, \Phi_{php'h'} \; \ldots$$

$$\Rightarrow \quad F\Phi_{ph} \, , \; F\Phi_{php'h'} \, , \ldots$$

non–orthogonal, correlated hilbertspace basis

Correlated Basis Fcts (CBF)

excited states

$$\psi \;\propto\; F\; e^{\frac{1}{2}U(t)}\; |\Phi_0\rangle \qquad\qquad \equiv \psi[c^{(1)}_{ph}\,,\; c^{(2)}_{pp'hh'}]$$

$\uparrow$ Jastrow correl. fct $\qquad$ $\uparrow$ Slater det

$$U(t) = \sum_{ph} c^{(1)}_{ph}(t)\, a^\dagger_p a_h + \sum_{pp'hh'} c^{(2)}_{pp'hh'}(t)\, a^\dagger_p a^\dagger_{p'} a_h a_{h'}$$

$$\Rightarrow \quad c^{(1)}\,\Phi_{ph}\,;\; c^{(1)}c^{(1)}\,\Phi_{php'h'}\,;\;\ldots\,;\quad c^{(2)}\,\Phi_{php'h'}\;\;\ldots$$

$$\Rightarrow \quad F\Phi_{ph}\,,\; F\Phi_{php'h'}\,,\ldots$$

non–orthogonal, correlated hilbertspace basis

action principle

$$\delta \left[S = \langle \psi \middle| H + H^{\text{ext}} + \frac{\hbar}{i} \frac{\partial}{\partial t} \middle| \psi \rangle \right] \stackrel{!}{=} 0$$

$\Rightarrow$ eqs of motion for $c^{(1)}$, $c^{(2)}$

linear response

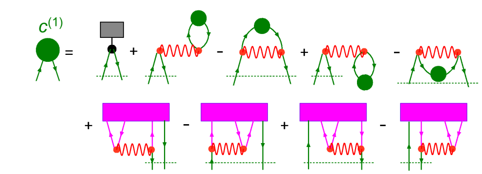
- assume **small** perturbation H^{ext}
- $F\Phi_0 =$ good descrition of the (unperturbed) ground state
- $\Rightarrow$ keep only **linear** terms in H^{ext}, $c^{(1)}$, $c^{(2)}$

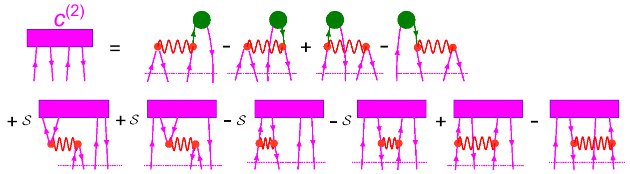
density

$$\rho = \frac{\langle \psi | \hat{\rho} | \psi \rangle}{\langle \psi | \psi \rangle} \approx \langle \hat{\rho} \rangle^0 + \delta \rho^{(1)} + \dots$$

$$\delta \rho^{(1)} =: \chi \, H^{\text{ext}}$$

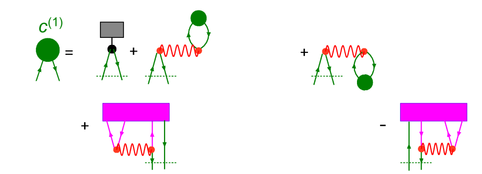
EOMs

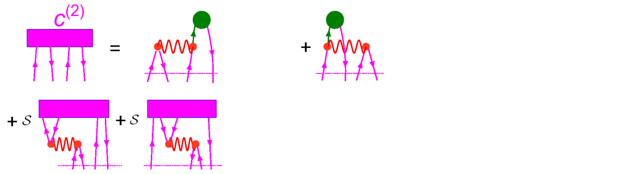




- retain (only) same terms as for bosons

EOMs





- retain (only) **same terms as for bosons**
    - in particular: omit exchange
    - and ,,similar” contributions (e.g. ladders)
    - fully correlated EOMs: product decoupling of overlap $\mathcal{N}^{(4)}$

EOMS: approximations

additional approximations:

1. assume **local** pair excitation operator $c^{(2)}_{php'h'} \longrightarrow c^{(2)}_{(p-h)\,(p'-h')}$
2. & replace $c^{(1)}_{ph} \longrightarrow c^{(1)}_{(p-h)}$ (only) in eq for $c^{(2)}$

$\widehat{=}$ equivalent to replacing these by their Fermi sea average

What does that mean?

Fermi sea average in Lindhard fct $\widehat{=}$ collapse *ph*-continuum into a single mode $\widehat{=}$,,SPA"=,,PPA"=,,CA" instead of RPA

$\Rightarrow$ pair excitations not treated as continuum

$\Rightarrow$ will need to be released for describing plasmon damping properly

response fct

$$\chi = \frac{\chi^0}{1 - v\chi^0}$$ standard RPA $c^{(1)} = 0,\ c^{(2)} = 0$ $\leftrightarrow$

$$\chi = \frac{\chi^0}{1 - V_{\mathrm{ph}}(q)\chi^0}$$ cRPA $c^{(1)} \neq 0,\ c^{(2)} = 0$ $\leftrightarrow$

$$\chi = \frac{\chi^s}{1 - V_{\mathrm{ph}}(q)\,\chi^s - \Gamma(q,\omega)}\,, \quad \chi^s = \ \ldots \quad \Gamma = \ \ldots$$ fluct pairs $c^{(1)} \neq 0,\ c^{(2)} \neq 0$

response fct

$$\chi = \frac{\chi^0}{1 - v\chi^0} \qquad \text{standard RPA} \quad c^{(1)} = 0,\ c^{(2)} = 0 \qquad \leftrightarrow$$

$$\chi = \frac{\chi^0}{1 - V_{\rm ph}(q)\chi^0} \qquad \text{cRPA} \quad c^{(1)} \neq 0,\ c^{(2)} = 0 \qquad \leftrightarrow$$

$$\chi = \frac{\chi^s}{1 - V_{\rm ph}(q)\,\chi^s - \Gamma(q,\omega)}, \qquad \chi^s = \ \ldots \qquad \Gamma = \ \ldots \qquad \text{fluct pairs} \quad c^{(1)} \neq 0,\ c^{(2)} \neq 0$$

$V_{\rm ph}(q) \ldots$
- ,,particle–hole interaction”. . . ,,diagram people”
- ,,pseudopotential” . . . ,,non–CondMatt people” (Pines)
- ,,local field correction” . . . ,,electron gas people”

identical for $\chi^{\rm cRPA}$ and $\chi^{\rm 2Pair}$!

Local Field Corrections (LFCs)

always possible: define some effective $\widetilde{V}(q,\omega)$ (electrons: v_q = Coulomb) via

$$\chi(q,\omega) =: \frac{\chi^0}{1-\widetilde{V}(q,\omega)\,\chi^0} =: \frac{\chi^0}{1-v_q(1-\mathcal{G})\,\chi^0}$$

approximate exact $\widetilde{V}(q,\omega) \rightarrow \widetilde{V}_{\text{approx}}(q)$

$$\widetilde{V}_{\text{approx}}(q) \leftrightarrow \begin{cases} \chi(q,\omega=0) & \text{static response} & \kappa \text{ sum rule} \\ \chi(q,\omega\to\infty) & \text{high frequency} & \omega^3 \text{ sum rule} \\ S(q)\propto\int d\omega\,\Im\mathrm{m}\chi & \text{static structure} & \omega^0 \text{ sum rule} \end{cases}$$

egas: 1957 Hubbard, 1968 STLS (Tas/Tomak → (06), Moudgil/Senatore/Saini (02)) and many others;

beyond static $\widetilde{V}(q)$ $\quad \dfrac{\chi^0}{1-\widetilde{V}(q,\omega)\,\chi^0} \quad \longleftarrow ? \longrightarrow \quad \dfrac{\chi^s}{1-V_{\text{ph}}(q)\,\chi^s-\Gamma(q,\omega)}$

self motion

Sjögren/Sjölander (78): dynamics of correlation hole surrounding a particle in classical fluids

$$\chi(q,\omega) = \frac{\chi^s}{1 + \left[X(q) - \frac{im\omega}{q^2} L(q,\omega)\right] \chi^s}$$

$X(q) = 1 - \frac{1}{S(q)}$ O.Z. direct c.f.

$L(q,\omega) = L[\chi, \chi^s]$ self. consist.

$\longrightarrow$ electron liquid: Neilson, Świerkowski, Sjölander, Szymański, PRB, (91)

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Holas (86): electron liquid sum rules: distinguish in Lindhard fct

$$-\chi^0 = \sum \frac{n^0_{\mathbf{k}+\mathbf{q}} - n^0_{\mathbf{k}}}{\omega - (t_{\mathbf{k}+\mathbf{q}} - t_{\mathbf{k}})} \quad \leftrightarrow \quad \sum \frac{n^{\mathrm{true}}_{\mathbf{k}+\mathbf{q}} - n^{\mathrm{true}}_{\mathbf{k}}}{\omega - (t_{\mathbf{k}+\mathbf{q}} - t_{\mathbf{k}})}$$

self motion

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$$-\chi^0=\sum\frac{n^0_{\mathbf{k}+\mathbf{q}}-n^0_{\mathbf{k}}}{\omega-(t_{\mathbf{k}+\mathbf{q}}-t_{\mathbf{k}})} \quad\leftrightarrow\quad \sum\frac{n^{\rm true}_{\mathbf{k}+\mathbf{q}}-n^{\rm true}_{\mathbf{k}}}{\omega-(t_{\mathbf{k}+\mathbf{q}}-t_{\mathbf{k}})}$$

$$\omega^3\Rightarrow\ \widetilde{V}(q\to 0,\infty):\ \boxed{v_q+\tfrac{4}{15}\varepsilon^{\rm pot}}+2(\varepsilon^{\rm kin}-\tfrac{3}{5}\varepsilon_{\rm F}) \quad\leftrightarrow\quad \boxed{v_q+\tfrac{4}{15}\varepsilon^{\rm pot}}$$

$$\omega^0\Rightarrow\ \widetilde{V}(q\to\infty,0):\ \tfrac{2}{3}(\varepsilon^{\rm kin}-\tfrac{3}{5}\varepsilon_{\rm F})+\boxed{v_q[\tfrac{1}{3}+\tfrac{2}{3}g(0)]} \quad\leftrightarrow\quad \boxed{v_q[\tfrac{1}{3}+\tfrac{2}{3}g(0)]}$$

self motion

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message:

$$\frac{\chi^0}{1-\widetilde{V}\,\chi^0} \;\leftarrow ? \rightarrow\; \frac{\chi^s}{1-\ldots}$$

though math. equivalent, some effects better in numerator (physics point of view!)

responsefct: details

$$\chi = \frac{\chi^s}{1 - V_{\rm ph}(q)\,\chi^s - \Gamma(q,\omega)}, \qquad \chi^s = \quad \ldots \qquad \Gamma = \quad \ldots$$

fluct pairs
$c^{(1)} \neq 0$, $c^{(2)} \neq 0$

$$\chi^s = \chi^0 - \chi^{0+}\chi^{0+}\left(\mathcal{A}^+ + \mathcal{A}^-\right)\frac{S_q}{S_q^0}$$

$$\chi^{0\pm} \equiv \sum \frac{n^0_{\mathbf{k}}\,(1 - n^0_{\mathbf{k+q}})}{\pm\omega - (t_{\mathbf{k+q}} - t_{\mathbf{k}})}$$

$$V_{\rm ph}(q) = \frac{q^2}{4m\,S_q{}^2} - \frac{q^2}{4m\,S_q^{0\,2}}$$

same as in cRPA
fct of static structure factor $S(q)$

$$\Gamma(q,\omega) = \frac{(S^2 + S^{0\,2})}{4SS^0}\,\chi^0\left(\mathcal{A}^+ + \mathcal{A}^-\right) - \frac{1}{2}\left(\chi^{0+} - \chi^{0-}\right)\left(\mathcal{A}^+ - \mathcal{A}^-\right) - \chi^{0+}\chi^{0-}\mathcal{A}^+\mathcal{A}^-$$

$$\mathcal{A}^\pm(q,\omega) = \sum_{q'}\left[W_3(\mathbf{q},\mathbf{q}',\mathbf{q}+\mathbf{q}')\right]^2 \mu^{\rm 0Pair}(\mathbf{q}',\mathbf{q}+\mathbf{q}',\pm\omega)$$

≈,,Chuck's formula" → vertex $W_3[S_q]$ pair Lindhard fct

time–dependent Hartree–Fock

cRPA $\widehat{=}$ tdHF with eom

$$\begin{pmatrix} (+\omega - \Delta t_{p,h})\,\delta_{\substack{pp' \\ hh'}} & 0 \\ 0 & (-\omega - \Delta t_{p,h})\,\delta_{\substack{pp' \\ hh'}} \end{pmatrix} \begin{pmatrix} c_{p'h'} \\ c^*_{p'h'} \end{pmatrix} = \begin{pmatrix} A_{ph,p'h'} & B_{php'h',0} \\ B_{p'h'ph,0} & A_{p'h',ph} \end{pmatrix} \begin{pmatrix} c_{p'h'} \\ c^*_{p'h'} \end{pmatrix}$$

with $A_{ph,p'h'} = V(p-h)\,\delta_{p-h,\pm(p'-h')} = B_{php'h',0}$

$p-h = q$ & skipping $\delta_{\ldots}$

time–dependent Hartree–Fock

cRPA $\widehat{=}$ tdHF with eom

$$\begin{pmatrix} (+\omega - \Delta t_{p,h}) & 0 \\ 0 & (-\omega - \Delta t_{p,h}) \end{pmatrix} \begin{pmatrix} c_{p'h'} \\ c^*_{p'h'} \end{pmatrix} = \begin{pmatrix} V(q) & V(q) \\ V(q) & V(q) \end{pmatrix} \begin{pmatrix} c_{p'h'} \\ c^*_{p'h'} \end{pmatrix}$$

with $A_{ph,p'h'} = V(p-h)\,\delta_{p-h,\pm(p'-h')} = B_{php'h',0}$

$p-h = q$ & skipping $\delta_{\dots}$

instead

$$= \begin{pmatrix} V(q) + \mathcal{A}(q,+\omega) & V(q) \\ V(q) & V(q) + \mathcal{A}(q,-\omega) \end{pmatrix} \begin{pmatrix} c_{p'h'} \\ c^*_{p'h'} \end{pmatrix}$$

$\Rightarrow\ \chi^{\text{2Pair}}$ with $S \to 1,\ S^0 \to 1$

Outline

input data

$$V_{\rm ph}(q) \;=\; \frac{q^2}{4m\,S_q{}^2} - \frac{q^2}{4m\,S_q^{0\,2}} \quad \leftarrow \; S(q) \in$$

ground state calcs
(take best available)

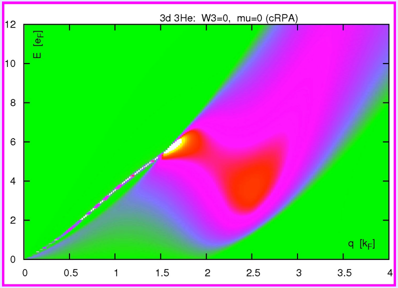
$$\mu^{0\rm Pair} \;=\; \begin{cases} \dfrac{S^0_{q'}\,S^0_{q''}}{\pm\omega - \varepsilon_{q'} - \varepsilon_{q''}} \\[2em] \sum \dfrac{n(1-n)\,n(1-n)}{\pm\omega - \ldots} \end{cases} \qquad \varepsilon_q = \frac{t_q}{S_q}$$

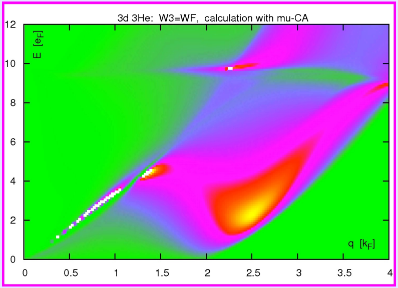
again $S(q)$
(Bogoliubov spectrum)

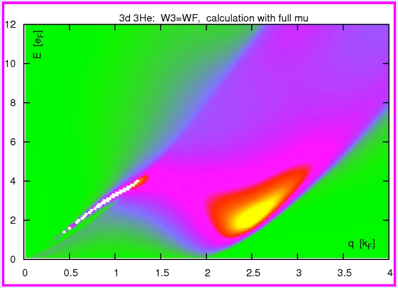
$$W_3 \;=\; \ldots \text{ (lengthy)} \;\; = \; W_3\left[S^0, S^{0(3)}, S\,\right]$$

again $S(q)$
no free parameters

results: 3d ^{3}He







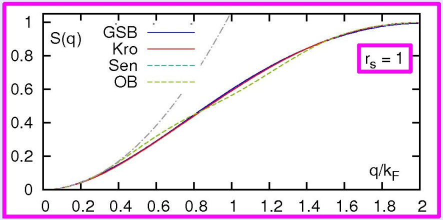
$S(q, \omega)$

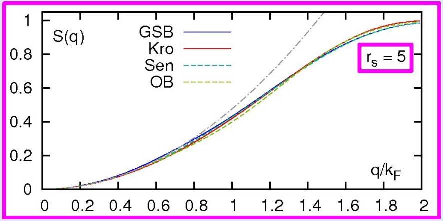
cRPA $\leftrightarrow \mu^{0\,\mathrm{CA}} \leftrightarrow \mu^{0\,\mathrm{2Pairs}}$

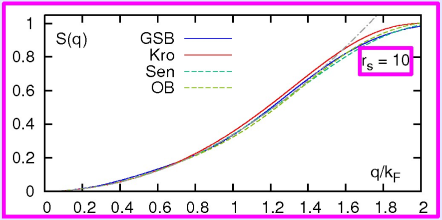
M Panholzer (07)

input: electrons

static structure factor S(q)







MC:

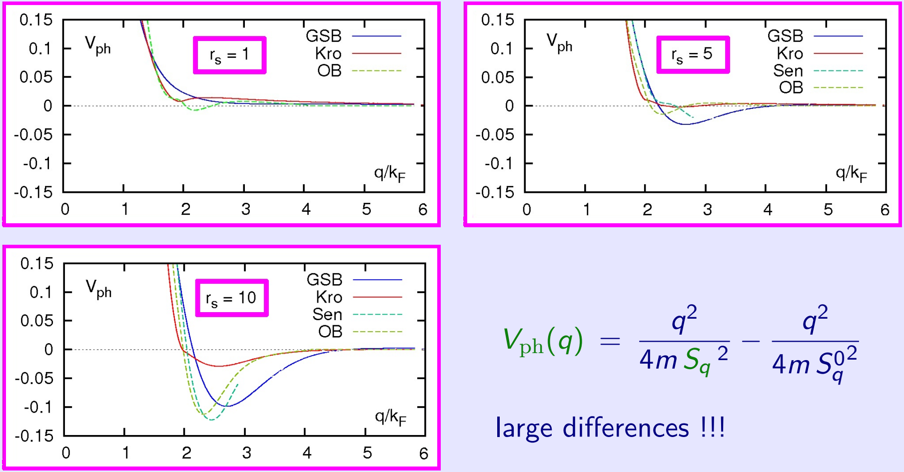
- Ortiz/Ballone (94)
- Senatore et al (92-98)
- Gori-Giorgi, Moroni, Bachelet (04)

FHNC:

- Krotscheck (78)

static V: electrons

particle-hole interaction $V_{\rm ph}(q)$

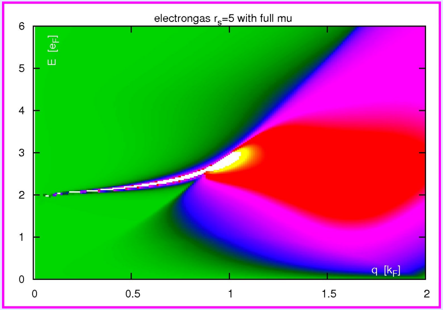


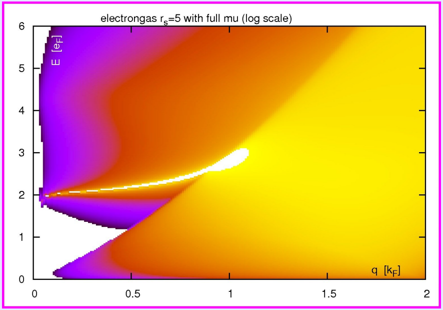
$$V_{\rm ph}(q) = \frac{q^2}{4m\, S_q{}^2} - \frac{q^2}{4m\, S_q^{0\,2}}$$

large differences !!!

results: $S(k,\omega)$ electrons

$r_s = 5$: double-plasmon visible (S^{FHNC})

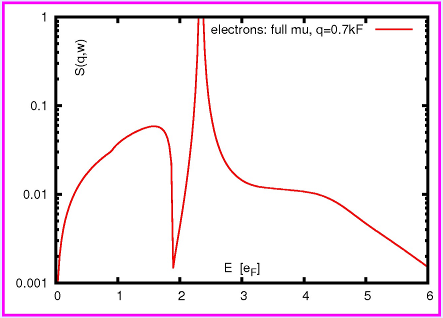


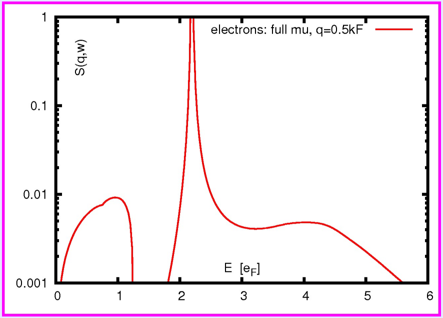


M. Panholzer, R. Holler (07)

results: $S(k,\omega)$ electrons (cont.)

$r_s = 5$: double-plasmon shoulder





$q = 0.5k_F$ $q = 0.7k_F$

summary / outlook

- fully microscopic description of denstity response fct χ of Fermions including pair–excitations

- exchange effects so far neglected

- parameter–free, input: static structure factor $S(q) \in$ ground state

- influence of the ,,pair continuum" $\leftrightarrow$ collective approx under investigation

Happy Birthday Chuck!