Physical interpretation of the Green's function in the interacting system. the quasiparticle concept

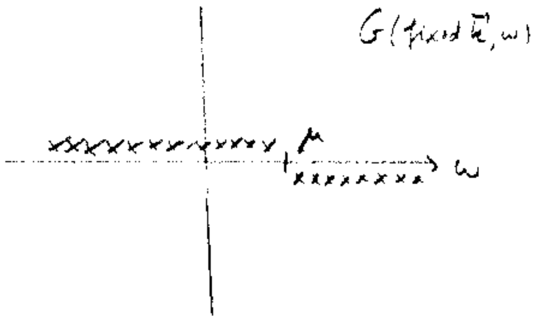
The basic idea underlying the concept of a quasiparticle is analyticity, with that we mean that states with the same symmetry (definite momentum, number of particles, spin, etc) can be adiabatically connected. If we think in terms of the analytic structure of the Green's function, we will find that the poles corresponding to low-energy excitations are still simple poles, but with different parameters compared to the noninteracting system $G^{(0)}(\vec{k},\omega) = \frac{1}{\omega - k^2/2m}$. This will enable us to even describe strongly interacting systems, of course provided there are no singularities e.g., due to phase transitions

Recall the Lehmann representation of the interacting Green's function:

$$G(\vec{k},\omega) = \sum_n \left(\frac{|\langle \Psi_n^{N+1} | a_{\vec{k}}^{\dagger} | \Psi_0^N \rangle|^2}{\omega - \mu - \varepsilon_n^{N+1} + i\eta} + \frac{|\langle \Psi_n^{N-1} | a_{\vec{k}} | \Psi_0^N \rangle|^2}{\omega - \mu + \varepsilon_n^{N-1} - i\eta} \right)$$

where $\varepsilon_n^{N+1} = E_n^{N+1} - E_0^N$ and $|\Psi_n^{N+1}\rangle$ are eigenstates of the interacting system $H|\Psi_n^{N+1}\rangle = E_n^{N+1}|\Psi_n^{N+1}\rangle$ with $N+1$ particles.

The pole structure of $G(\vec{k},\omega)$



and spectral densities $\quad \rho^+(\vec{k},\omega) = \sum_n |\langle \Psi_n^{N+1} | a^\dagger_{\vec{k}} | \Psi_0^N \rangle|^2 2\pi\, \delta(\omega - \varepsilon_n^{N+1})$,

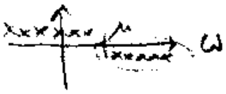
$$\rho^-(\vec{k},\omega) = \sum_n |\langle \Psi_n^{N-1} | a_{\vec{k}} | \Psi_0^N \rangle|^2 2\pi\, \delta(\omega - \varepsilon_n^{N-1})$$

and $\rho(\vec{k},\omega) = \theta(\omega)\, \rho^+(\vec{k},\omega) + \theta(-\omega)\, \rho^-(\vec{k},-\omega)$

$$\Rightarrow \quad G(\vec{k},\omega) = \int_0^\infty \frac{d\omega'}{2\pi} \left[\frac{\rho^+(\vec{k},\omega')}{\omega-\mu-\omega'+i\eta} + \frac{\rho^-(\vec{k},\omega')}{\omega-\mu+\omega'-i\eta} \right]$$

For this lecture, we consider $\omega > \mu$. Thus we study the propagation of particles. The arguments are the same for $\omega < \mu$, and will lead to no new effects.

For $\omega > \mu$, the only poles in $G(\vec{k},\omega)$ are from the ρ^+ piece



$$G(\vec{k},\omega>\mu) = \int_0^\infty \frac{d\omega'}{2\pi} \frac{\rho^+(\vec{k},\omega')}{\omega-\mu-\omega'+i\eta} = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\rho^+(\vec{k},\omega')}{\omega-\mu-\omega'+i\eta}$$

$\rho^+ = 0$ for $\omega < \varepsilon_0^{N+1}$ and we can extend the integral for free

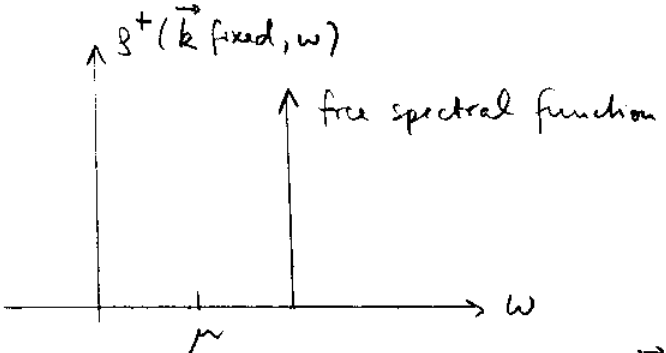
Using $\frac{1}{\omega' \pm i\eta} = P\frac{1}{\omega'} \mp i\pi\delta(\omega')$ leads to a (dispersion) relation

$$\mathrm{Im}\, G(\vec{k}, \omega > \mu) = -\frac{1}{2}\rho^+(\vec{k}, \omega - \mu > 0)$$

For a free particle ($k > k_F$)

$$\mathrm{Im}\, G^{(0)}(\vec{k}, \omega > \mu) = \mathrm{Im}\, \frac{1}{\omega - \frac{k^2}{2m} + i\eta} = -\pi\,\delta\left(\omega - \frac{k^2}{2m}\right)$$

$$\Rightarrow \rho^+_{(0)} = 2\pi\,\delta\left(\omega - k^2/2m\right)$$



$\rho^+(\vec{k}$, as fn of $\omega)$

Therefore, the spectral function describes the distribution of energies in the system when a particle with momentum $\vec{k}$ is added. Analogously, $\rho^-(\vec{k}, \omega < \mu)$ ... when a hole with momentum $\vec{k}$ is added (= a particle with $\vec{k}$ removed). For free particles, the momentum state $\vec{k}$ is also an eigenstate of the Hamiltonian $\Rightarrow \rho^+_{(0)} \sim \delta(\omega - k^2/2m)$.

How does the spectral function change in the interacting system? We have the general expression:

$$\rho^+(\vec{k},\omega) = \sum_n |\langle \Psi_n^{N+1} | a^\dagger_{\vec{k}} | \Psi_0^N \rangle|^2 \, 2\pi \, \delta(\omega - \varepsilon_n^{N+1})$$

What are the allowed intermediate states?

- need N+1 particles in total
- momentum conservation demands $\hat{P} |\Psi_n^{N+1}\rangle = \vec{k} |\Psi_n^{N+1}\rangle$ so in fact $|\Psi_n^{N+1}\rangle = |\Psi_{\vec{k}}^{N+1}\rangle$ and momentum labels intermediate states

(• additionaly: spin, charge, .. conservation)

Expand $|\Psi_{\vec{k}}^{N+1}\rangle$ in a complete set of states with the above symmetries:

will be clear later

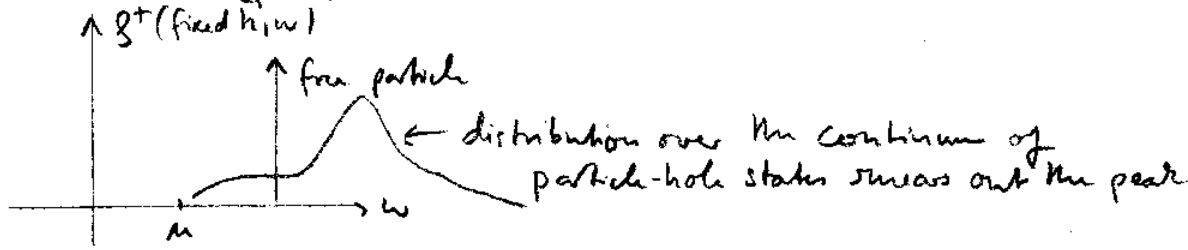
$$|\Psi_{\vec{k}}^{N+1}\rangle = Z_{\vec{k}}^{1/2} \underbrace{a^\dagger_{\vec{k}} |\Psi_0^N\rangle}_{N+1 \text{ part.}} + \sum_{\vec{p},\vec{p}'} \alpha_{\vec{k},\vec{p},\vec{p}'} \underbrace{a^\dagger_{\vec{p}} \, a_{\vec{p}'} \, a^\dagger_{\vec{k}+\vec{p}'-\vec{p}} |\Psi_0^N\rangle}_{\substack{N+1 \text{ part} \\ \text{momentum } \vec{k} \text{ o.k.}}}$$

$$+ \text{ 3 particle-2 hole} + \text{ 4 particle-3 hole} + \ldots$$

where $Z_{\vec{k}}$, $\alpha_{\vec{k},\vec{p},\vec{p}'}$ are the expansion coefficients.

The interaction kicks particles from below the Fermi surface to above. There is a continuum of momenta $\sum_{\vec{p},\vec{p}'}$ available for these intermediate states. The added particle therefore has a wide distribution of energies.

And we might guess, that the spectral function in the interacting system looks something like this



We will now show that this is indeed the form of the spectral function. We will study this in a schematic model. We also go back to our diagrammatical approach, in contrast to the above expansion of the wave function.

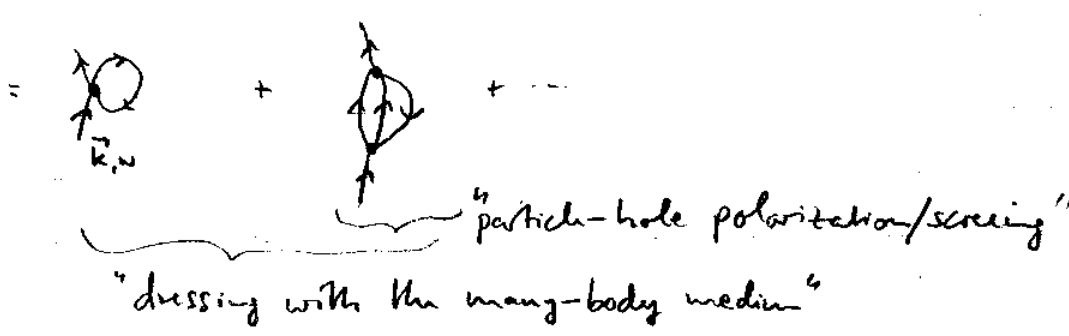
The many-body physics is contained in the proper self-energy $\Sigma^*(\vec{k},\omega)$ and from Dyson's equation we have

$$G(\vec{k},\omega) = \frac{1}{\omega - \varepsilon_{\vec{k}} - \Sigma^*(\vec{k},\omega) + i\eta}$$

can drop $i\eta$, since $\mathrm{Im}\,\Sigma^* < 0$ at second order

The essential features of Σ^* arise already in the first two orders of perturbation theory.

$$\Sigma^*(\vec{k},\omega) = \Sigma^{*(1)}(\vec{k},\omega) + \Sigma^{*(2)}(\vec{k},\omega) + \cdots$$



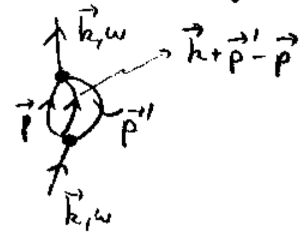
$$\Sigma^{*(1)} = \frac{k_F^2}{2m}(g-1)\frac{4}{3\pi}(k_F a_s) \sim k_F^3$$

(recall
$-i\,\mathrm{Tr}\,G(\vec{x},t;\vec{x},t^+) = \rho(\vec{x}) = \frac{k_F^3}{3\pi^2}$
for homogeneous systems)

Thus $\Sigma^{*(1)}$ is $\vec{k}$ and ω independent.
We absorb it into $\varepsilon_{\vec{k}}$ and define $E_0(\vec{k}) = \varepsilon_{\vec{k}} + \Sigma^{*(1)}$.

$$\Rightarrow \quad G = \frac{1}{\omega - E_0(\vec{k}) - \Sigma^{*(2)}(\vec{k},\omega)}$$

For the dilute Fermi system with C_0

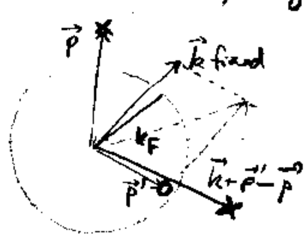
$\Sigma^{*(2)} =$


$$\sim \frac{1}{2}\int\frac{d^3\vec{p}}{(2\pi)^3}\int\frac{d^3\vec{p}'}{(2\pi)^3}\,\Theta(k_F-p')\,\Theta(p-k_F)$$

sym factor

$$\times\,\Theta(|\vec{k}+\vec{p}'-\vec{p}|-k_F)\,\frac{C_0^2}{\omega+\varepsilon_{p'}-\varepsilon_p-\varepsilon_{k+p'-p}+i\eta}$$

A momentum configuration, which contributes, is given by



× particles
o hole

[+ the 2 hole - 1 particle contribution from the different time ordering
$\Sigma^{*(2)}(2h\,1p)$ has only poles for $\omega<\mu$
$\Rightarrow$ contributes to g^-. see Negele + Orland, p. 250
We still are interested in $\omega>\mu$]

The double-integral is still cumbersome, but the essential features are

1) continuum of poles in the intermediate state, just like $\frac{\quad\mu\quad}{xxxxxx}\,\omega$ for $\omega>\mu$

2) Scattering of particles near the Fermi surface is inhibited by Pauli blocking of the occupied states

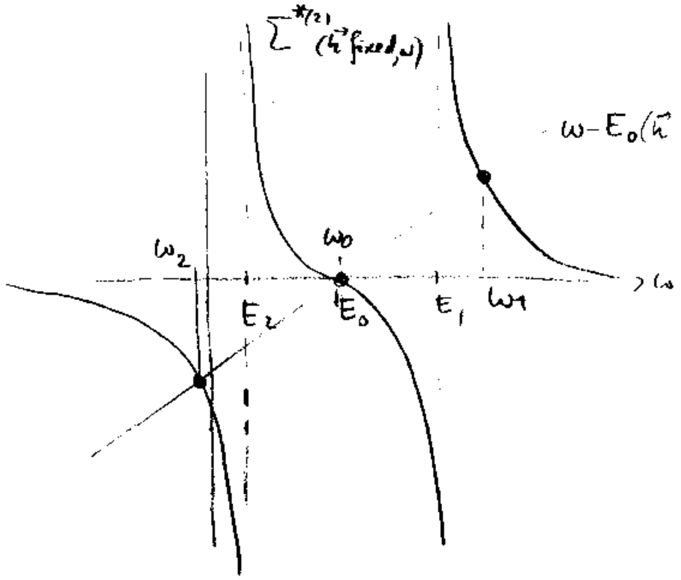
We model the behavior of $\sum^{*(2)}(\vec{k},\omega)$ as a sum of equally spaced (try randomly spaced in the notebook, e.g.) poles

$$\sum^{*(2)}(\vec{k},\omega) \approx \sum_{n=0}^{N} \frac{\lambda^2}{\omega-(E_1-\Delta E\cdot n)}$$

↑ some spacing

Start with only two poles $\sum^{*(2)}(\vec{k},\omega) = \frac{\lambda^2}{\omega-E_1} + \frac{\lambda^2}{\omega-E_2}$

with $E_1 > E_0 > E_2$ and $E_1 - E_2 = \Delta E$ and we dropped the $i\eta$



The zero's of the interacting Green function are given by $\omega - E_0(\vec{k}) = \sum^{*(2)}(\vec{k},\omega)$. The graphical solution for fixed $\vec{k}$ is given by the intersection of $\omega - E_0$ and $\sum^{*(2)}(\omega)$. They are denoted by $\omega_2, \omega_0, \omega_1$, see Figure.

In terms of the ω_i, the Green's function can be written as

$$G(\vec{k},\omega) = \sum_{i=0}^{2} \frac{z_i(\vec{k})}{\omega - \omega_i(\vec{k}) + i\eta}$$

Where the residues $z_i(\vec{k})$ are given by

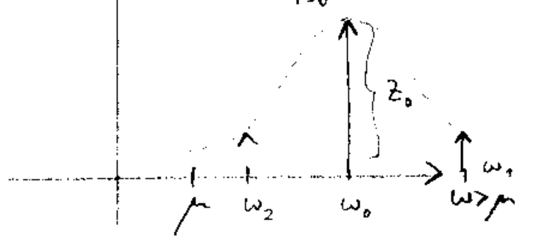
$$z_i(\vec{k}) = \lim_{\omega\to\omega_i(\vec{k})} \left(\omega-\omega_i(\vec{k})\right) G(\vec{k},\omega) = \lim_{\omega\to\omega_i(\vec{k})} (\omega-\omega_i(\vec{k})) \frac{1}{\omega - E_0(\vec{k}) - \sum^{*(2)}(\vec{k},\omega)}$$

Both numerator and denominator vanish, then the $z_i(\vec{k})$ may be obtained through l'Hospital's rule

$$z_i(\vec{k}) = \frac{1}{1 - \left.\frac{\partial \Sigma^{*(2)}(\vec{k},\omega)}{\partial \omega}\right|_{\omega=\omega_i(\vec{k})}} = \frac{1}{1 + \left(\frac{\lambda^2}{(\omega_i(\vec{k})-E_1)^2} + \frac{\lambda^2}{(\omega_i(\vec{k})-E_2)^2}\right)} < 1.$$

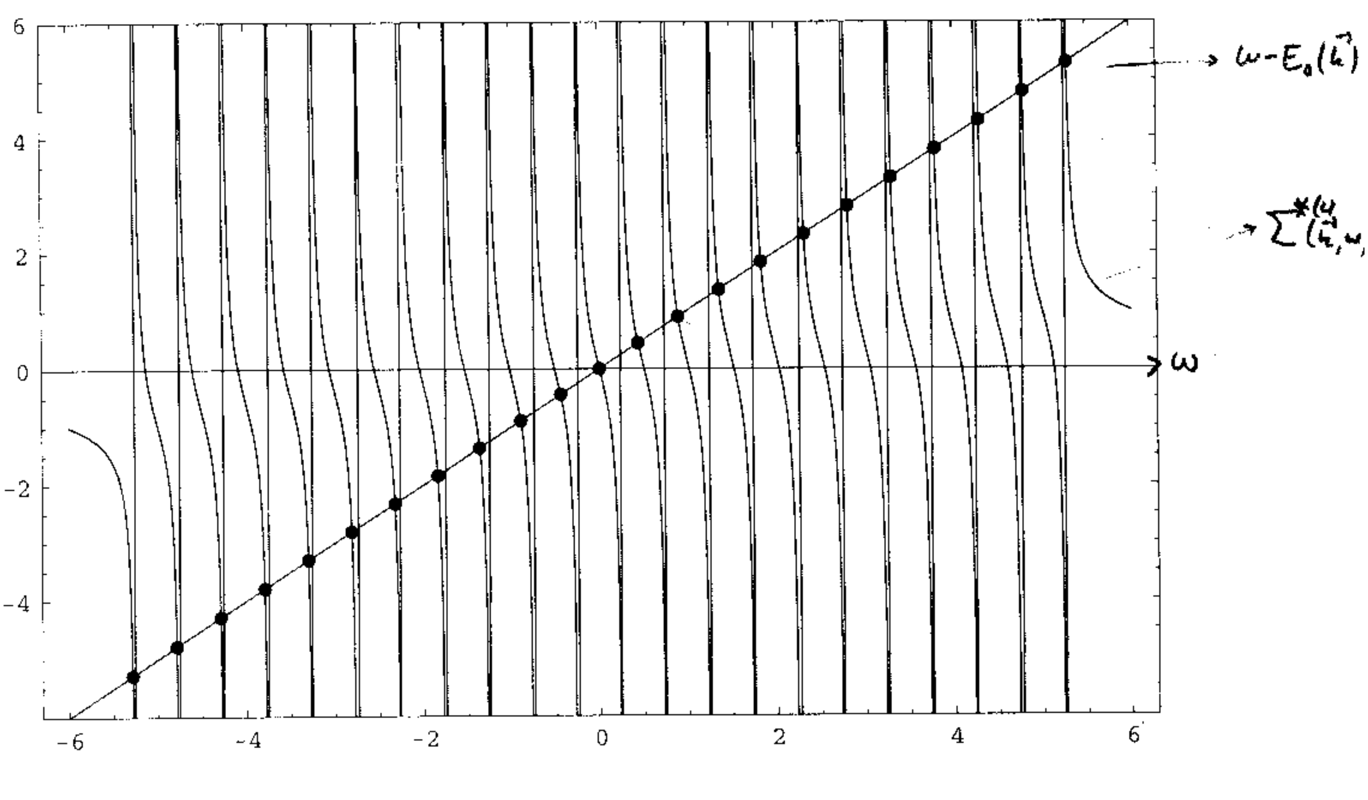
$z_i(\vec{k})$ is maximal, when $(\omega_i(\vec{k})-E_1)^2$ and $(\omega_i(\vec{k})-E_2)^2$ are maximal, this is the case for ω_0, whereas ω_1 and ω_2 have larger residues. A plot of the spectral function is given by

$$\rho^+(\vec{k},\omega) = \sum_{i=0}^{2} 2\pi\, z_i(\vec{k})\, \delta(\omega - \omega_i(\vec{k}))$$

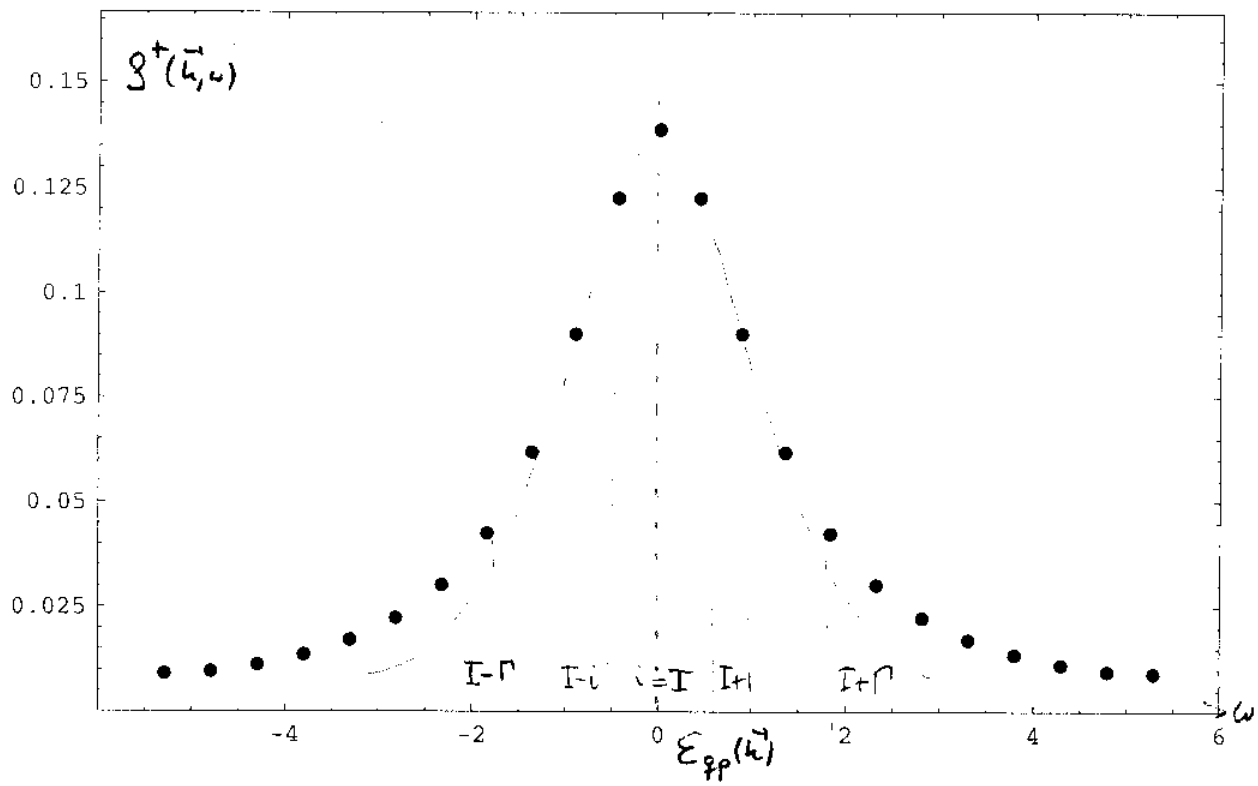


$\Longrightarrow$ strength is distributed over particle-hole intermediate states, leads to a smeared peak

Use Mathematica, to include more poles in $\Sigma^{*(2)}$:



And the spectral function[1)]



- The position of the peak defines the energy of the quasiparticle $\varepsilon_{qp}(\vec k) \neq \varepsilon_{\vec k}$ (free particle energy)
- The quasiparticle excitation is given by the linear combination of eigenstates $\omega_i(\vec k)$ around the peak, $|i-I| \leq \Gamma$
- The quasi particle strength is defined by $Z_{qp} = \sum_{|i-I|\leq\Gamma} z_i(\vec k)$
- The background of the remaining modes are far apart in energy ω and thus decay faster. (We will discuss this further in one of the following lectures.)
- We have well defined quasiparticles in the infinite system, if Z_{qp} is finite as $N\to\infty$, $V\to\infty$, $\frac{N}{V}=\varrho$ fixed.

1) The spectral weights obey a sum rule, see Negele + Orland p. 244, in our schematic model $\sum_{\text{all } i} z_i(\vec k) = 1$.

We now parametrize the quasiparticle part of the interacting Green's function by

$$\boxed{G_{qp}(\vec{k},\omega) = \frac{Z_{\vec{k}}}{\omega - \mathcal{E}_{qp}(\vec{k}) + \frac{i}{\tau_{\vec{k}}}} \;, \quad \omega > \mu \quad \begin{matrix} \omega \gtrsim \mu \\ |\vec{k}| \simeq k_F \end{matrix}}$$

Why is this reasonable?

$$\Rightarrow \quad \varrho^+(\vec{k}, \omega - \mu > 0) = -2 \operatorname{Im} G_{qp}(\vec{k}, \omega > \mu)$$

$$= -2 \operatorname{Im} \frac{Z_{\vec{k}}\left(\omega - \mathcal{E}_{qp}(\vec{k}) - i/\tau_{\vec{k}}\right)}{(\omega - \mathcal{E}_{qp}(\vec{k}))^2 + \frac{1}{\tau_{\vec{k}}^2}}$$

$$= \frac{2 Z_{\vec{k}}/\tau_{\vec{k}}}{(\omega - \mathcal{E}_{qp}(\vec{k}))^2 + \frac{1}{\tau_{\vec{k}}^2}}$$

= Lorentzian peak in the spectral function, a typical peak shape.

width of the quasiparticle

We will derive that $\frac{1}{\tau_{\vec{k}}} \sim (\mathcal{E}_{qp}(\vec{k}) - \mu)^2$, i.e., the quasiparticles are long-lived in the vicinity of the Fermi surface $\mathcal{E}_{qp}(\vec{k}) \simeq \mu$.

Coming back to the introductory statements, we have demonstrated in a general model that the analytic structure of the interacting Green's function at low-energies has the same qualitative behavior as a free particle — a simple pole — with different "parameters" however. In the remainder, we will discuss experimental evidence for this quasiparticle picture in nuclear physics as well as the physical content of the "parameters" in the qp Green's function

By comparison of G_{qp} and the Lehmann representation, we observe

$$\boxed{z_{\vec{k}} = |\langle\Psi_{\vec{k}}^{N+1}|\, a_{\vec{k}}^{\dagger}\, |\Psi_0^{N}\rangle|^2 = \frac{1}{1-\frac{\partial\Sigma}{\partial\omega}\Big|_{\omega=\varepsilon_{qp}(k^2)}} \Rightarrow z_{k_F} = \frac{1}{1-\frac{\partial\Sigma}{\partial\omega}\Big|_{\substack{\omega=\mu\\ k=k_F}}}}$$

thus the $z_{\vec{k}}^{1/2}$ on p. 183

"z - factor" on the Fermi surface

Physical definition z_{k_F}: overlap of the ground state wave function of a system of interacting $N+1$ (or $N-1$) fermions with momentum $\vec{k}$ with the wave function of N interacting particles and a bare particle of momentum $\vec{k}$.

or: single quasiparticle with momentum $\vec{k}$ to be in a single particle state with momentum $\vec{k}$

Evidence of quasiparticle excitations in heavy nuclei

Study of $3s_{1/2}$ (proton) charge distributions in ^{206}Pb versus ^{205}Tl (= single proton quasihole in ^{206}Pb)

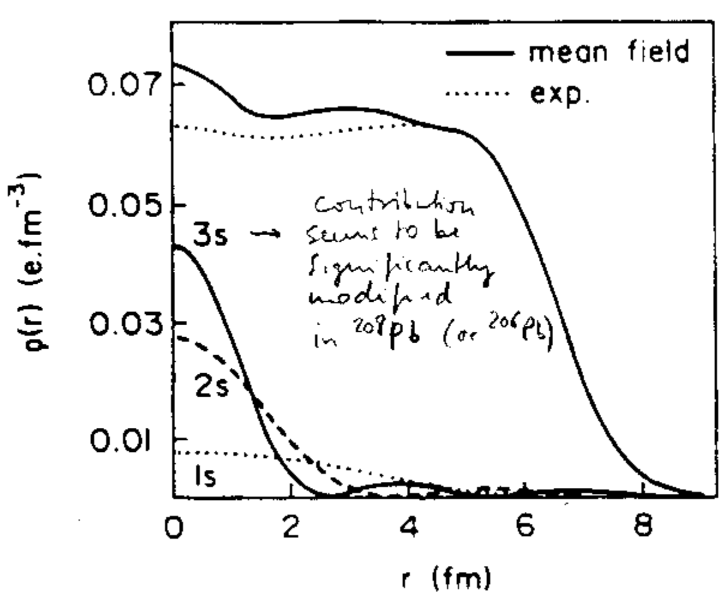


Figure 7: *Charge density of ^{208}Pb. The contributions of the 1s, 2s and 3s proton orbits to the total charge density are mean field predictions [Fr77,De80].*

The $p\,3s_{1/2}$ (radial quant. #) is the last filled level before shell closure (= Fermi surface) to 82 protons.

The Figure shows the contributions of $1s_{1/2}$, $2s_{1/2}$, $3s_{1/2}$ protons to the total charge density, assuming all proton levels up to $3s_{1/2}$ are filled, all higher ones are empty.

The total charge density in nuclei can be probed by means of elastic electron scattering. The elastic cross section depends on the Fourier transform of the charge distribution. For details, see B. Frois and I. Sick (Eds): "Modern Topics in e⁻ Scattering", World Scientific 1991, 352–392, where I took the figures from as well.

$$\left(\frac{d\sigma}{d\Omega}\right)_{eA\to eA} = \left[\frac{Z\alpha\cos\theta/2}{2E\sin^2\theta/2}\right]^2 \frac{1}{1+\frac{2E}{M}\sin^2\frac{\theta}{2}} \; |F(\vec{q})|^2$$

with $F(\vec{q}) = \frac{1}{Ze}\int \rho(\vec{r})\, \underbrace{e^{i\vec{q}\cdot\vec{r}}}_{\sim j_0(qr)\text{ for spherically sym. charge distribution}} d^3\vec{r}$

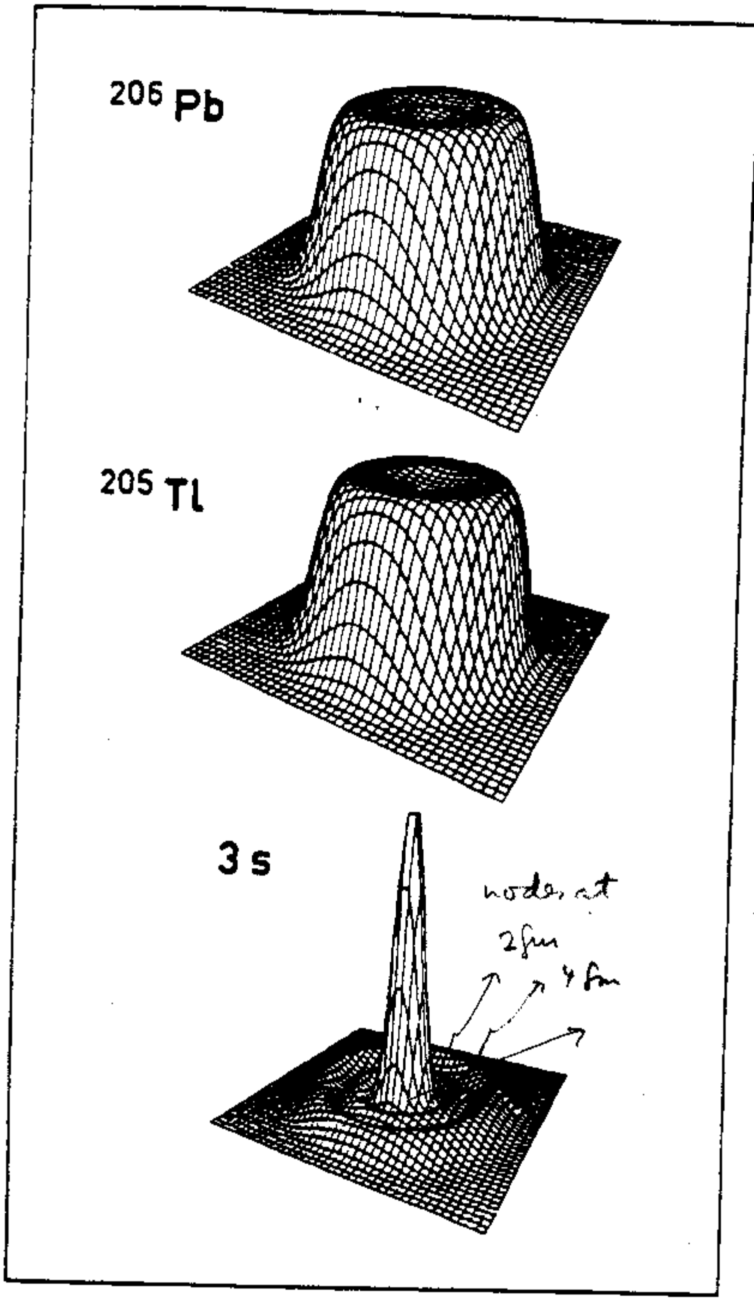
The charge density difference between ^{206}Pb and ^{205}Tl directly probes the $3s_{1/2}$ protons, since the $3s_{1/2}$ has a unique shape, see Fig. 9, while the p, d, .. orbits peak at the surface of the nucleus.

Therefore, the effect of the $3s_{1/2}$ proton shows up in the ratio of cross sections of ^{205}Tl to ^{206}Pb as a peak, see Fig. 10.

Elastic electron-nucleus scattering confirms our picture of the quasiparticle!

In the next lecture, we will construct an effective theory among quasiparticles, Landau's Fermi liquid theory, where we will consider the excitation of quasiparticles created by $\alpha^+_{\vec{k}} = z_{\vec{k}}^{1/2}\, a^+_{\vec{k}} + \ldots$ and calculate the resulting physical properties.

due to ω-dependence of Σ
the rest is multi particle-hole.



⇒ has largest overlap with the Bessel function $j_0(qr)$ at $q_0 = 2\ fm^{-1}$

Figure 9: *Two-dimension contours of the charge density distributions of ^{206}Pb, ^{205}Tl and of the 3s orbit. The amplitude of the 3s distribution is multiplied by 2).*

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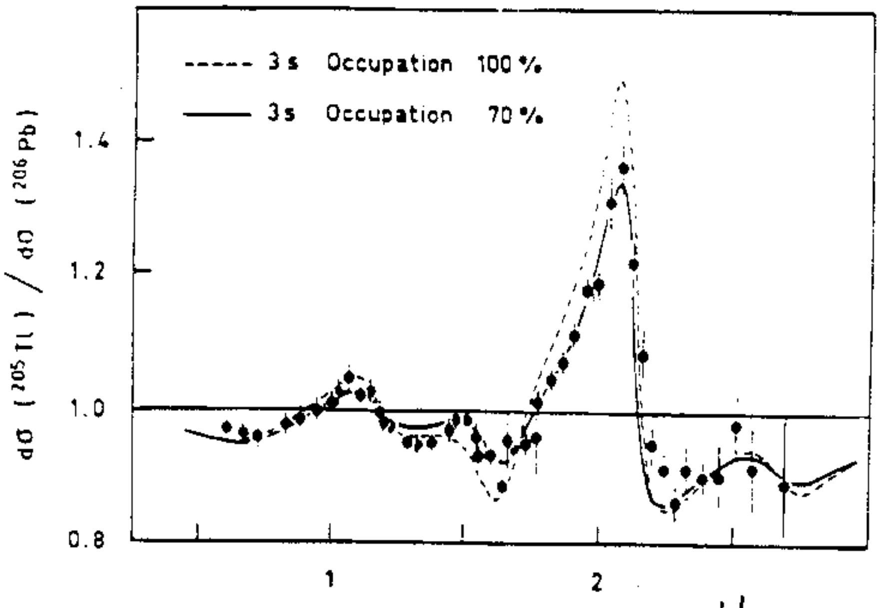

$q_0 \approx 2 fm^{-1}$!

typical for a proton quasihole

⇒ ~70% single proton

~30% higher multi-particle-hole excitations

⇒ shape of $3s_{1/2}$ proton orbit is observed! Thus, single particle picture valid.

Figure 10: *The ratio of elastic cross sections from* ^{205}Tl *and* ^{206}Pb *[Ca82, Eu78]. The curves are mean field predictions with a finite range density dependent interaction [De80,CS72].*

But, fragmentation of strength, see above, as in our quasiparticle picture.

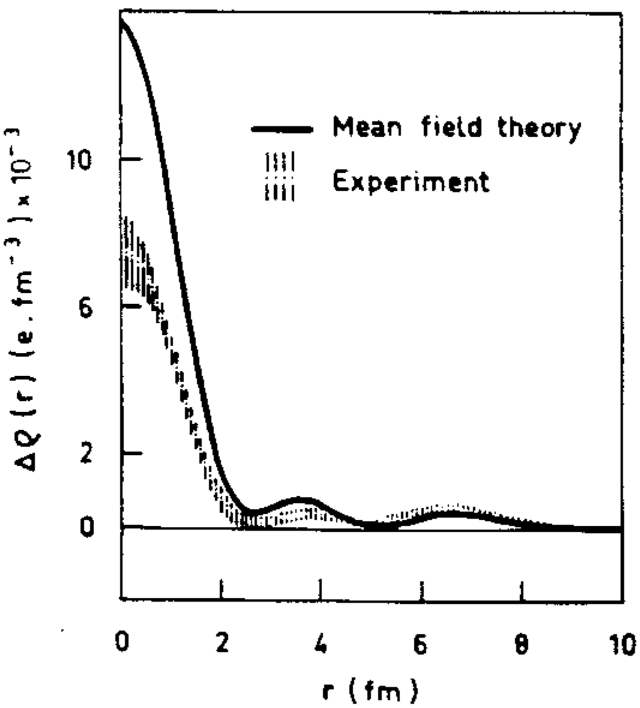

Figure 11: *The charge density difference of* ^{206}Pb *and* ^{205}Tl *[Ca82,De80].*