Quasiparticle weights and many-body states

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Choose an orthonormal basis of one-particle states $\phi_n(x)$. We will work in this basis with an N electron system with ground state $|0,N\rangle$ of energy E_0^N and with $N\pm 1$ electron excited states $|m,N\pm 1\rangle$ of energy $E_m^{N\pm 1}$. The Green's matrix in the Källen-Lehmann representation is given by

$$G_{nm}(\omega) = \sum_p \frac{f_p(n)f_p(m)^*}{\omega - \epsilon_p + i0^+} + \sum_h \frac{f_h(n)f_h(m)^*}{\omega - \epsilon_h - i0^+}\,.$$

The particle or "conduction" (p) and hole or "valence" (h) states are just labels for many-body states for $N+1$ and $N-1$ electrons:

$$f_p(n) = \langle 0,N|\hat{a}_n|p,N+1\rangle \quad , \quad f_h(n) = \langle 0,N|\hat{a}_n^\dagger|h,N-1\rangle\,,$$

$$\epsilon_p = E_p^{N+1} - E_0^N \quad , \quad \epsilon_h = E_0^N - E_h^{N-1}\,.$$

The amplitudes $f_j(n)$ are overlaps of many-body and single-particle type states: *e.g.*

$$|f_p(n)|^2 = |\langle p,N+1|\left\{\hat{a}_n^\dagger|0,N\rangle\right\}|^2$$

is the amount of the single-particle type state obtained by adding an electron in state n to the ground-state in the actual many-body excited state p. We have the simple sum rules

$$\begin{aligned}
\sum_p |f_p(n)|^2 &= \langle 0,N|\hat{a}_n\hat{a}_n^\dagger|0,N\rangle = 1 - \langle 0,N|\hat{a}_n^\dagger\hat{a}_n|0,N\rangle \\
\sum_h |f_h(n)|^2 &= \langle 0,N|\hat{a}_n^\dagger\hat{a}_n|0,N\rangle \\
\sum_p |f_p(n)|^2 + \sum_h |f_h(n)|^2 &= 1
\end{aligned}$$

which directly relates to the occupancy of the state n. The off diagonal generalizations tell us about the ground-state one-particle density matrix, *e.g.*

$$\sum_h f_h(n)f_h(m)^* = \langle 0,N|\hat{a}_n^\dagger\hat{a}_m|0,N\rangle\,.$$

At any rate, these sum rules tell us the "amount" of an added or subtracted single particle in all of the many-body Hilbert space which is a simple question with a simple answer.

What we really want is the converse: to what extent does an actual many-body excitation look like it is made from various combinations of adding single electrons to $|0, N\rangle$? Here we are taking the many-body ground state and adding an electron in a single-particle state to it which does not give us an eigenstate in general. We want the sum

$$S_p = \sum_n |f_p(n)|^2 = \sum_n \langle 0, N|\hat{a}_n|p, N+1\rangle\langle p, N+1|\hat{a}_n^\dagger|0, N\rangle$$

This is not very easy to understand as written. To see the role of S_j , set $n = m$ and sum over all n for the Green's function matrix to get

$$\sum_n G_{nn}(\omega) = \sum_p \frac{S_p}{\omega - \epsilon_p + i0^+} + \sum_h \frac{S_h}{\omega - \epsilon_h - i0^+} \,.$$

If S_p is very close to unity, then we can say that the many-body excited state looks like some linear combination of single-electron states added to the ground state (and by doing a unitary transform we can change that to a single electron state). In the usual quasiparticle approximation, we assume the S_j are unity for our one-particle band states and zero otherwise. Note that there are *many* more many-body states than single-particle states (the latter always can be counted with a discrete integer index at some crystal momentum whereas the former become a continuum above some energy).

To make more progress, we use an alternate form of the Green's matrix. The Dyson equation gives us an energy dependent "Hamiltonian". Specifically,

$$G_{nm}(\omega) = [\omega I - H(\omega)]^{-1}_{nm} \,,$$

where all the matrices are in the ϕ_n basis, and $H(\omega)$ is our "Hamiltonian" matrix from Dyson's equation: $H = T + U_{ion} + U_{Hartree} + \Sigma(\omega)$. We diagonalize $H(\omega)$ at a given ω with eigenvectors V and eigenvalues e and label the eigenstates with a discrete index α:

$$G_{nm}(\omega) = \sum_\alpha \frac{V(\omega)_{n\alpha} V(\omega)^{-1}_{\alpha m}}{\omega - e_\alpha(\omega)} \,. \tag{1}$$

We do not assume orthonormal eigenvectors for $H(\omega)$ so we must use of the inverse matrix $V(\omega)^{-1}$. This particular form is more useful than choosing left and right eigenvectors.

We find solutions to the mathematical equation

$$\omega = e_\alpha(\omega) \,.$$

for a given a fixed α over complex ω. Let a solution be $\bar{\omega}_\alpha$, $\bar{\omega}_\alpha = e_\alpha(\bar{\omega}_\alpha)$. Good physical solutions are quasiparticles which have small imaginary parts for $\bar{\omega}_\alpha$ (i.e., long lifetimes) and are isolated from other solutions. When scanning over real ω, this means that $G(\omega)$ will have a sharp and narrow peak in the form of an isolated pole around $\mathrm{Re}(\bar{\omega}_\alpha)$.

Close to such a pole, we can isolate the contribution from $\bar{\omega}_\alpha$ from the remaining background,

$$G_{nm}(\omega) = \frac{Z_\alpha V(\bar{\omega}_\alpha)_{n\alpha} V(\bar{\omega}_\alpha)^{-1}_{\alpha m}}{\omega - \bar{\omega}_\alpha} + B_\alpha(\omega)\,,$$

where the background $B_\alpha(\omega)$ is a smooth and analytic function of ω about $\bar{\omega}_\alpha$ coming from other states in the sum in Equation (1) as well as subleading terms from expanding about the α term itself about $\bar{\omega}_\alpha$. The quasiparticle renormalization factor is defined as

$$Z_\alpha \equiv \left(1 - \frac{de_\alpha(\bar{\omega}_\alpha)}{d\omega}\right)^{-1}\,.$$

Setting $n = m$ and summing over n gives a simple pole and a new background about $\bar{\omega}_\alpha$,

$$\sum_n G_{nn}(\omega) = \frac{Z_\alpha}{\omega - \bar{\omega}_\alpha} + C_\alpha(\omega)\,.$$

Comparing to our previous result, we see that

$$Z_\alpha \cong S_j$$

when we can make a good identification of a quariparticle state. To the extent that $Z_\alpha \approx 1$, we can replace our many-body excited states by simple states coming from adding electrons into single-particle states above the ground state.