Orthogonality catastrophe

CMT Journal Club, given by John Chalker

May 29th, 2015 Thomas Veness

References

- P. W. Anderson, Phys. Rev. Lett. **18**, 1049 (1967)
- K. D. Schotte and U. Schotte, Phys. Rev. **182**, 479 (1969)

Moral: Hilbert space is a big place, but Fock space is really big!

The ideas covered here date back to the 1960s, when people were thinking about the Kondo effect. The material relates to X-ray edge singularities, but has applications to many other topics that are still of theoretical and experimental relevance.

1 Simple background

We wish to consider an overlap between two vectors in a vector space. If we pick two random chosen unit vectors from an N-dimensional complex vector space $\mathbb{C}^N$, $|\psi\rangle$, $|\varphi\rangle$, then we can see that

$$\overline{|\langle\psi|\varphi\rangle|^2} = \frac{1}{N}. \tag{1}$$

This therefore means hat for an infinite-dimensional vector space, that two randomly chosen vectors are almost surely orthogonal. In single-particle physics, it is easy to choose vectors in a way that certainly *isn't* random. It is, however, difficult to choose two vectors with a finite overlap in a many-body system. To see that, consider an N-boson wavefunction (for simplicity), specifically of the form

$$\Psi(r_1, \ldots, r_N) = \prod_{i=1}^{N} \psi(r_i), \qquad \Phi(r_1, \ldots, r_N) = \prod_{i=1}^{N} \varphi(r_i), \tag{2}$$

then

$$|\langle\Psi|\Phi\rangle|^2 = |\langle\psi|\varphi\rangle|^{2N} \tag{3}$$

and therefore, for any distinct states, the overlap is exponentially small in N. When comparing many-body wavefunctions, we must therefore ask whether the fall-off is small or not. The interesting thing about the orthogonality catastrophe is that the overlap is intermediate between the two scenarios above.

2 X-ray edge problem

If we consider a metal with an impinging X-ray, this can excite a core electron and cause photoelectric emission. Considering the absorption spectrum, the non-interacting picture would lead us to believe that we have an onset of absorption with a step-function at $\omega = E_f + E_{\text{core}}$. If we wish to go beyond this picture, then we must worry about different interactions. Landau Fermi liquid theory might lead us to believe that we can ignore the interactions between the conduction electrons, but there are also interactions due to the core hole acting as a potential for the other electrons. The question we wish to address, therefore, is: *what is the effect of the core hole on the final state?* In term of Fermi's Golden Rule, we will see that the onset is there, but that this is a *matrix element* effect that causes a distinctly different kind of onset to that of the non-interacting picture.

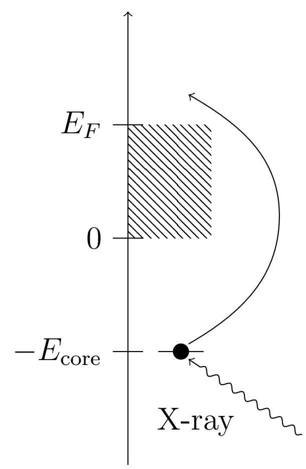

Figure 1: Schematic view of the problem under consideration

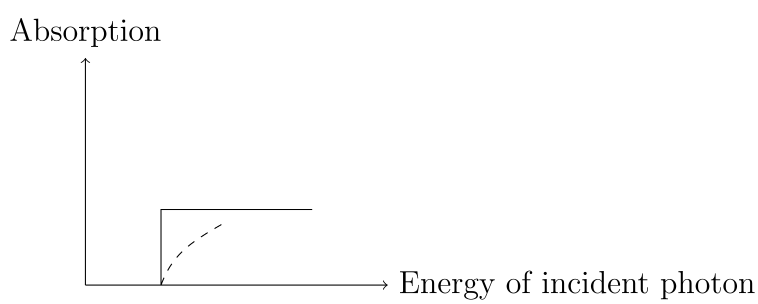

Figure 2: The naïve expectation (solid line) of the absorption in the X-ray edge problem, compared to what is observed (dashed line)

To understand how the core hole changes the Fermi see, we consider the overlap between the ground state of the system without the hole and the ground state with a hole i.e.

$$|\langle O_{\text{hole}}|O_{\text{no hole}}\rangle|^2 \tag{4}$$

If this is very small, then so will be the matrix element when using Fermi's Golden Rule. These overlaps are, in principle, easy to think about, as they are a determinant of an $M \times M$ matrix of overlaps, as the wavefunctions are constructed in terms of Slater Determinants i.e.

$$|\langle O_{\text{hole}}|O_{\text{no hole}}\rangle|^2 = |\det M|^2, \qquad M_{kl} = \langle \psi_k|\varphi_l\rangle. \tag{5}$$

There are two possibilities according to the strength of the potential: if we can produce a bound state, then this would be $O(1/\sqrt{V})$ for each element. In three dimensions, we need a sufficiently deep potential to form a bound state. If we consider expansion the wavefunction in the presence of a hole in terms of the basis of states of those without a hole i.e.

$$\varphi_l = c_{lk}\psi_k \tag{6}$$

then we can project out the piece above the Fermi energy and rescale i.e.

$$|\langle O_{\text{hole}}|O_{\text{no hole}}\rangle|^2 = \prod_l \left(1 - \sum_{E_k>E_F} |c_{kl}|^2\right) (\text{det of matrix of unit vectors})^2 \tag{7}$$

We can therefore see that

$$|\langle O_{\text{hole}}|O_{\text{no hole}}\rangle|^2 \leq \prod_l \left(1 - \sum_{E_k>E_F} |c_{kl}|^2\right) \leq e^{-S} \tag{8}$$

where

$$S = \sum_{E_l<E_F} \sum_{E_k>E_f} |c_{lk}|^2, \tag{9}$$

where we have used that $(1-x) \leq e^{-x}$, if $x > 0$. So, how do we evaluate this sum? Suppose we have a Hamiltonian

$$H_0\varphi_k = \varepsilon_k\varphi_k \tag{10}$$

$$(H_0 + V\delta(r))\psi_l = \omega_l\psi_l \tag{11}$$

where $\psi_l = c_{lk}\varphi_k$, then projecting this onto φ_k, we see that

$$c_{lk} = \frac{V\varphi_k^*(0)\varphi_k(0)}{\omega_l - \varepsilon_k} \tag{12}$$

and therefore

$$\psi_l(0) = \sum_k c_{lk}\varphi_k(0) = V\sum_k \frac{\varphi_k^*(0)\varphi_k(0)}{\omega_l - \varepsilon_k}\psi_l(0) \tag{13}$$

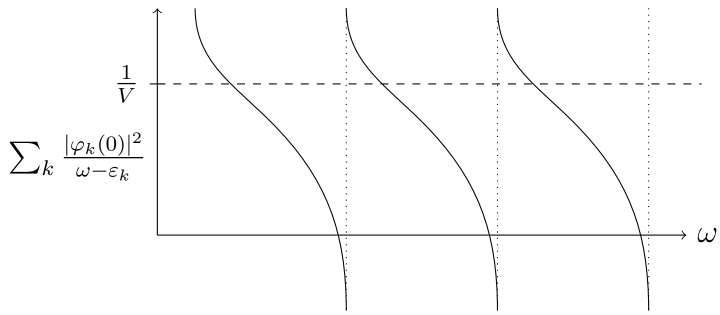

Figure 3: A graphical representation of solutions to eq. (14)

Which implies that

$$\frac{1}{V} = \sum_k \frac{|\varphi_k(0)|^2}{\omega_l - \varepsilon_k} \tag{14}$$

Up to an overall normalisation, we have that

$$c_{lk} = \mathcal{N} \frac{\varphi_k^*(0)}{\omega_l - \varepsilon_k} \tag{15}$$

and, using the normalisation of $\sum_k |c_{lk}|^2 = 1$, we see

$$\mathcal{N}^{-2} = \sum_k \frac{|\varphi_k|^2}{(\omega_l - \varepsilon_k)^2} \sim \frac{1}{N} \tag{16}$$

We can now evaluate the sum approximately:

$$S = \sum_{E_l > E_F} \sum_{E_k > E_F} \mathcal{N}^2 \frac{|\varphi|^2}{(\omega - \varepsilon)^2} \tag{17}$$

$$\int^{E_F} \mathrm{d}\varepsilon \int_{E_F} \mathrm{d}\omega \frac{1}{(\omega - \varepsilon)^2} \tag{18}$$

$$\int_0 \mathrm{d}\varepsilon \int_0 \mathrm{d}\omega \frac{1}{(\omega + \varepsilon)^2} \tag{19}$$

$$= \int_0 \frac{\mathrm{d}s}{s} \tag{20}$$

The upper limit of integration is determined by the bandwidth. We can see that there is a logarithmic divergence in the system size, which means that there is a power-law fall-off of the overlap.

3 Where did the weight go?

As the states become orthogonal in the thermodynamic limit, due to each Hamiltonian being furnished with a complete set of eigenstates, the overlap of the initial state must be distributed somehow in the spectrum of the perturbed Hamiltonian. We would like to know how the weight of the hole-free state has been distributed among these states. If we consider the spectral function

$$S(\omega) = |\langle \alpha_{\text{hole}} | O_{\text{no hole}} \rangle|^2 \delta(\varepsilon_\alpha - \omega), \tag{21}$$

then this will answer precisely this question. We can first consider the Fourier transform

$$\widetilde{S}(t) = \int \mathrm{d}\omega \, S(\omega) e^{i\omega t} = \langle O_{\text{no hole}} | \alpha \rangle e^{it\varepsilon_\alpha} \langle \alpha | O_{\text{no hole}} \rangle = \langle O_{\text{no hole}} | e^{iH_{\text{hole}} t} | O_{\text{no hole}} \rangle \tag{22}$$

3.1 Bosonisation

This problem is most easily attacked via bosonisation. We will not cover this comprehensively, by any means, but will simply utilise some results. We have bosonic operators b_q, $b_q^\dagger$, which create electron-hole pairs on the Fermi sea obeying the usual algebra

$$[b_q, b_{q'}^\dagger = \delta_{q,q'} \tag{23}$$

Under the assumption of the linearity of the free spectrum, we have

$$H_0 = \hbar\nu = \sum_{k>0} b_k^\dagger b_k \tag{24}$$

$$H_{\text{hole}} = V \psi^\dagger(0)\psi(0) = \frac{V}{L} \sum_{kq} c_k^\dagger c_q = \frac{V}{\sqrt{L}} \sum_k \sqrt{k}(b_k^\dagger + b_k) \tag{25}$$

Completing the square in the total Hamiltonian

$$H_0 + H_{\text{hole}} = \sum_k k(b_k^\dagger + \frac{V}{\sqrt{Lk}})(b_k + \frac{V}{\sqrt{Lk}}) + \text{const.} \tag{26}$$

Defining $\beta_k = b_k + \frac{V}{\sqrt{Lk}}$, we have that

$$H = \sum_k k \beta_k^\dagger \beta_k \tag{27}$$

and

$$b_k | O_{\text{no hole}} \rangle = 0 \Rightarrow \beta_k | O_{\text{no hole}} \rangle = \frac{V}{\sqrt{Lk}} | O_{\text{no hole}} \rangle \tag{28}$$

This implies that $|O_{\text{no hole}}\rangle$ is a coherent state and we can therefore calculate

$$\widetilde{S}(t) = e^{F(t)}, \qquad F(t) = \sum_k \frac{V^2}{kL}(e^{itk} - 1) \sim -\frac{V^2}{2\pi} \ln(1 - \frac{it}{\alpha}) \tag{29}$$