Embedded Cluster Boundary Condition: Background

Kondo problem - cluster/environment logarithmic-derivative matching

Objective: Effect of an impurity atom on the density of states of jellium.

Method: Match a numerical wave function in the core to a plane wave outside.

\[
\left[-\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{2m}{\hbar^2} V(r) + \frac{l(l+1)}{r^2} \right] \psi_k(r) = \frac{k^2 \psi_k(r)}{U(r)} \quad (r \leq R_0)
\]  

where

\[ E = \frac{\hbar^2 k^2}{2m} \]  

\[ \psi(r) = \psi_k(r) Y_{lm}(\theta, \phi) \]  

Match the logarithmic derivative of the cluster state,

\[ L_-(k) = \frac{\psi_k(r_0)}{\psi_k(r_0)} \]  

to the environment (plane-wave) state,

\[ \psi_k(r) = j_0(kr) - C(k) n_e(kr) \quad (r_0 \leq r \leq R) \]

where

\[ C(k) = \frac{j_1(kR)}{n_e(kR)} \]

so that \( \psi_k(kR) = 0 \) at the universe boundary.
Note

\[ L_+(k) = \frac{U_k(r_0^+)}{U_k(r_0^+)} = \frac{j_0'(kr_0) - C(k) \eta_0(kr_0)}{j_0(kr_0) - C(k) \eta_0(kr_0)} \quad (7) \]

Marching the cluster and environment logarithmic derivatives,

\[ L_+(k) = L_-(k) \quad (8) \]

we get, from Eq (7),

\[ j_0'(kr_0) - C(k) \eta_0(kr_0) \]
\[ j_0(kr_0) - C(k) \eta_0(kr_0) \]

\[ = L_-(k) \]

or

\[ [j_0'(kr_0) - C(k) \eta_0(kr_0)] L_-(k) = j_0(kr_0) - C(k) \eta_0(kr_0) \]

\[ C(n' - n_L) = j' - j_L \]

\[ \frac{j_0'(kr_0) - j_0(kr_0) L_-(k)}{\eta_0'(kr_0) - \eta_0(kr_0) L_-(k)} = \frac{j_0(kR)}{\eta_0(kR)} \]

\[ C(k) = \frac{j_0(kR)}{\eta_0(kR)} \quad (9) \]

The eigenenergies, \( k \), are determined to satisfy the secular equation, (9).

Note that asymptotically,

\[ C(k) = \frac{j_0(kR)}{\eta_0(kR)} \to \frac{\pm \sin(x - \frac{3\pi}{2})}{-\frac{1}{x} \cos(x - \frac{3\pi}{2})} \bigg|_{x = kR} = -\tan(\beta R - \frac{3\pi}{2}) \quad (kR \to \infty) \quad (10) \]

so that Eq (9) has solutions every \( \pi/R \), i.e., perturbation to free \( k_{\alpha}^{(1)} \) (note only \( j_0(kr) \) is non-singular at origin)

\[ k_{\alpha}^{(1)} = \frac{\ell \pi}{2} = n\pi \]

or

\[ k_{\alpha}^{(1)} = (n + \frac{\ell}{2}) \frac{\pi}{R} \quad (11) \]
A rapid variation in \([i^2 \delta(k) - i^2(k) L_-(k)] / [\eta_0(k) - \eta_i(k) L_-(k)]\) - resonance - gives rise to nonuniform distribution of the perturbed eigenenergies, \(k_n\).
Open boundary condition for scattering states


\[ \psi_R(x) = e^{ikx} + t(k) e^{-ikx} \quad (x \leq -\frac{L}{2}) \]  \hfill (1)

\[ \psi_R(x) = t(k) e^{ikx} \quad (x \geq \frac{L}{2}) \]  \hfill (2)

(Open boundary condition: Specify 0th & 1st derivatives)

\[ \psi(-L/2) = e^{-ikL/2} + re^{ikL/2} \]  \hfill (3)

\[ \psi'(-L/2) = ik(e^{ikL/2} - r e^{ikL/2}) \]  \hfill (4)

From Eqs. (3) & (4), we can eliminate \( r \):

\[ re^{ikL/2} = \psi(-L/2) - e^{-ikL/2} = -\frac{\psi'(-L/2)}{ik} + e^{-ikL/2} \]

\[ \psi(-L/2) + \frac{\psi'(-L/2)}{ik} = 2e^{-ikL/2} \quad (0th \& 1st \text{ derivative relation}) \]  \hfill (5)

Or

\[ \psi + \frac{1}{ik} \frac{\psi_2 - \psi_0}{2\Delta x} = 2e^{-ikL/2} \]

\[ 2i\Delta x \psi + \psi_2 - \psi_0 = 4i\Delta x e^{-ikL/2} \]

\[ \therefore \psi_0 = 2i\Delta x \psi + \psi_2 - 4i\Delta x e^{-ikL/2} \]
(Open boundary condition and Lippmann-Schwinger equation)

The open boundary condition, Eqs. (1) & (2), is equivalent to using the Lippmann-Schwinger equation,

\[ \Psi(x) = \Psi_0(x) + \int dx' G_0(x, x'; E) \Psi(x') \]  

(10)

where

\[ E = \hbar^2 k^2 / 2m \]  

(11)

\[ \Psi_0(x) = e^{ikx} \]  

(12)

\[ G_0(x, x'; E) = \frac{dk}{2\pi} \frac{e^{ik(x-x')}}{E - \hbar^2 k^2 / 2m} \]  

(13)

\[ \rightarrow \text{check!} \]