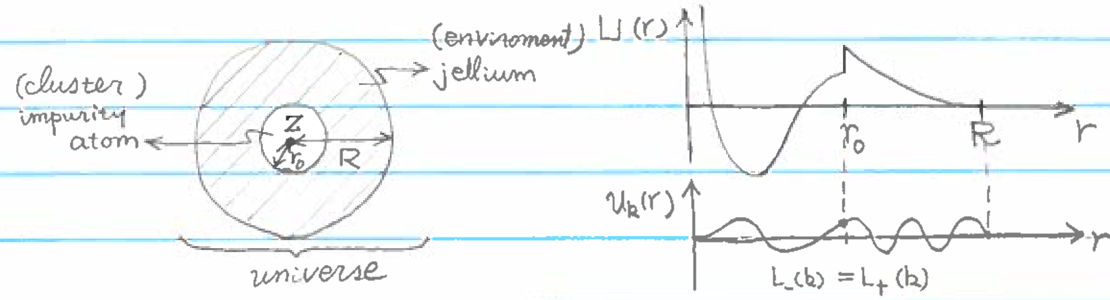
Embedded Cluster Boundary Condition: Background

7/6/03

— 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.

$$\Big[\underbrace{-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{2m}{\hbar^2}V(r) + \frac{\ell(\ell+1)}{r^2}}_{U(r)}\Big] u_k(r) = k^2 u_k(r) \quad (r \le r_0) \qquad (1)$$

where

$$E = \hbar^2 k^2/2m \qquad (2)$$

$$\psi(\mathbf{r}) = u_k(r) Y_{\ell m}(\theta, \varphi) \qquad (3)$$

0th & 1st derivative

Match the logarithmic derivative of the cluster state,

$$L_-(k) = \frac{u_k'(r_0 - 0)}{u_k(r_0 - 0)} \qquad (4)$$

first derivative

to the environment (plane-wave) state,

$$u_k(r) = j_\ell(kr) - C(k)\, n_\ell(kr) \quad (r_0 \le r \le R) \qquad (5)$$

where

$$C(k) = \frac{j_\ell(kR)}{n_\ell(kR)} \qquad (6)$$

so that $u_k(kR) = 0$ at the universe boundary.

Note

$$L_+(k) = \frac{u_k'(r_0+0)}{u_k(r_0+0)} = \frac{j_\ell'(kr_0) - C(k)\, n_\ell'(kr_0)}{j_\ell(kr_0) - C(k)\, n_\ell(kr_0)} \tag{7}$$

Matching the cluster and environment logarithmic derivatives,

$$L_+(k) = L_-(k) \tag{8}$$

we get, from Eq. (7),

$$\frac{j_\ell'(kr_0) - C(k)\, n_\ell'(kr_0)}{j_\ell(kr_0) - C(k)\, n_\ell(kr_0)} = L_-(k)$$

or

$$[j_\ell(kr_0) - C(k)\, n_\ell(kr_0)]\, L_-(k) = j_\ell'(kr_0) - C(k)\, n_\ell'(kr_0)$$

$$c(n' - nL) = j' - jL$$

$$\therefore \quad \boxed{\frac{j_\ell'(kr_0) - j_\ell(kr_0)\, L_-(k)}{n_\ell'(kr_0) - n_\ell(kr_0)\, L_-(k)} = C(k) = \frac{j_\ell(kR)}{n_\ell(kR)}} \tag{9}$$

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

Note that asymptotically

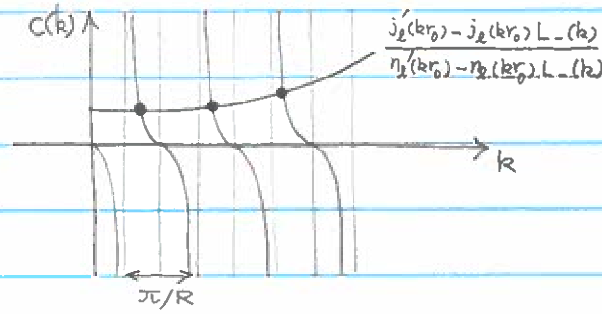
$$C(k) = \frac{j_\ell(kR)}{n_\ell(kR)} \to \left.\frac{\frac{1}{x}\sin(x - \frac{\ell\pi}{2})}{-\frac{1}{x}\cos(x - \frac{\ell\pi}{2})}\right|_{x=kR} = -\tan(kR - \tfrac{\ell\pi}{2}) \quad (kR \to \infty) \tag{10}$$

so that Eq. (9) has solutions every π/R, i.e., perturbation to free $k_n^{(0)}$ (note only $j_\ell(kr)$ is non-singular at origin)

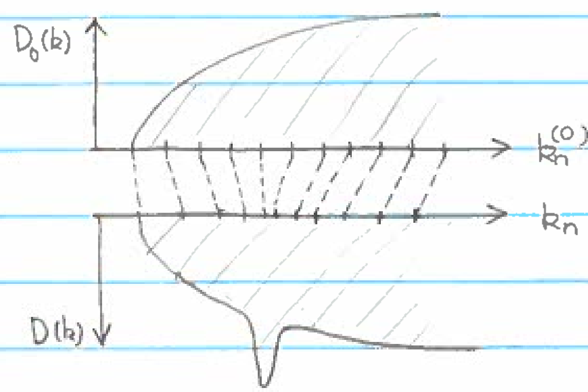
$$k_n^{(0)} R - \frac{\ell\pi}{2} = n\pi$$

or

$$k_n^{(0)} = (n + \frac{\ell}{2})\frac{\pi}{R} \tag{11}$$

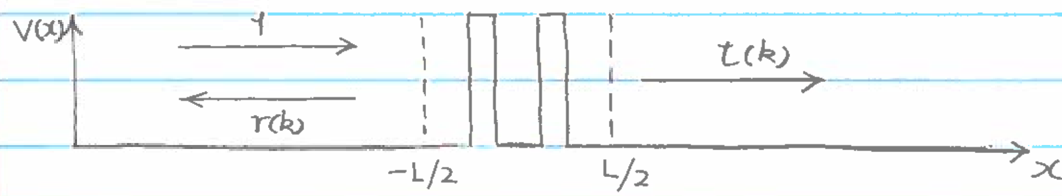


A rapid variation in $[j_\ell'(kr_0) - j_\ell(kr_0)L_-(k)]/[\eta_\ell'(kr_0) - \eta_\ell(kr_0)L_-(k)]$ — resonance — gives rise to nonuniform distribution of the perturbed eigenenergies, k_n.



— Open boundary condition for scattering states.

[A.M. Kriman, N.C. Kluksdahl, D.K. Ferry, PRB 36, 5953 ('87); N.C. Kluksdahl, A.M. Kriman, D.K. Ferry, C. Ringhofer, PRB 39, 7720 ('89)]



For $k > 0$ (similar but reflected for $k<0$)

$$\begin{cases} \psi_k(x) = e^{ikx} + r(k)\, e^{-ikx} & (x \le -\frac{L}{2}) \quad (1) \\ \psi_k(x) = t(k)\, e^{ikx} & (x \ge \frac{L}{2}) \quad (2) \end{cases}$$

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

$$\begin{cases} \psi(-L/2) = e^{-ikL/2} + r\, e^{ikL/2} & (3) \\ \psi'(-L/2) = ik\left(e^{-ikL/2} - r\, e^{ikL/2}\right) & (4) \end{cases}$$

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

$$r e^{ikL/2} = \psi(-L/2) - e^{-ikL/2} = -\frac{\psi'(-L/2)}{ik} + e^{-ikL/2}$$

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

$\simeq$ logarithmic derivative

Or

$$\psi_1 + \frac{1}{ik}\,\frac{\psi_2 - \psi_0}{2\Delta x} = 2e^{-ikL/2}$$

$$2ik\Delta x\, \psi_1 + \psi_2 - \psi_0 = 4ik\Delta x\, e^{-ikL/2}$$

$$\therefore \psi_0 = 2ik\Delta x\, \psi_1 + \psi_2 - 4ik\Delta x\, e^{-ikL/2}$$

(Open boundary condition and Lippmann-Schwinger equation)

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

$$\psi(x) = \psi_0(x) + \int dx' G_0(x,x';E)\psi(x') \tag{10}$$

where

$$\begin{cases} E = \hbar^2 k^2/2m & (11) \\ \psi_0(x) = e^{ikx} & (12) \\ G_0(x,x';E) = \displaystyle\int \frac{dk}{2\pi} \frac{e^{ik(x-x')}}{E-\hbar^2k^2/2m} & (13) \end{cases}$$

→ check!