Yosida / Varma–Yafet Variational Singlet for the Kondo Model

1. Model and Notation

$$H \;=\; \sum_{k\sigma} \epsilon_k \, c^\dagger_{k\sigma} c_{k\sigma} \;+\; J\, \boldsymbol{S}_{\rm imp}\!\cdot\!\boldsymbol{s}_0, \qquad \boldsymbol{s}_0 = \frac{1}{2}\sum_{kk'\alpha\beta} c^\dagger_{k\alpha}\boldsymbol{\sigma}_{\alpha\beta}c_{k'\beta}, \quad J>0.$$

* D : half-bandwidth of a flat conduction band, $\rho_0 = 1/(2D)$. * $|\mathrm{FS}\rangle$: filled Fermi sea ($\epsilon_k \le 0$). * $\boldsymbol{S}_{\rm imp}$: impurity spin–$\frac{1}{2}$.

Throughout we set the Fermi energy to zero.

2. Trial State (Singlet Ansatz)

$$\boxed{|\Psi[\phi]\rangle = \frac{1}{\sqrt{2}}\Big(|{\Uparrow}\rangle_{\rm imp}\sum_k \phi_k\, c^\dagger_{k\downarrow} - |{\Downarrow}\rangle_{\rm imp}\sum_k \phi_k\, c^\dagger_{k\uparrow}\Big)\,|\mathrm{FS}\rangle}$$

- ϕ_k are complex variational amplitudes ($\sum_k |\phi_k|^2 = 1$).
- The state is an *exact spin singlet:* $\big(\boldsymbol{S}_{\rm imp} + \boldsymbol{s}_0\big)^2\,|\Psi\rangle = 0$.
- Physically: one conduction electron is promoted above the Fermi sea into orbital $\phi(\boldsymbol{r}) = \sum_k \phi_k \psi_k(\boldsymbol{r})$ and binds antiferromagnetically to the impurity.

3. Norm

$$\langle\Psi|\Psi\rangle = \frac{1}{2}\sum_{kk'}\phi^*_k\phi_{k'}\;\underbrace{\langle \mathrm{FS}|c_{k\downarrow}c^\dagger_{k'\downarrow}|\mathrm{FS}\rangle}_{=\,\delta_{kk'}\theta(-\epsilon_k)} + \frac{1}{2}\sum_{kk'}\phi^*_k\phi_{k'}\;\underbrace{\langle \mathrm{FS}|c_{k\uparrow}c^\dagger_{k'\uparrow}|\mathrm{FS}\rangle}_{=\,\delta_{kk'}\theta(-\epsilon_k)} = \sum_{\epsilon_k>0}|\phi_k|^2 = 1,$$

because only *unfilled* ($\epsilon_k > 0$) orbitals can be added.

4. Energy Expectation

Kinetic part. Only the promoted electron contributes:

$$E_{\rm kin} = \sum_{\epsilon_k>0} |\phi_k|^2\,\epsilon_k.$$

Exchange part. Using $\boldsymbol{S}_{\rm imp}\cdot\boldsymbol{s}_0 = \frac{1}{2}\Big(\mathcal{P}_{\rm triplet} - \frac{3}{4}\Big)$, a total singlet yields $\langle \boldsymbol{S}_{\rm imp}\cdot\boldsymbol{s}_0\rangle = -\frac{3}{4}$. Hence

$$E_{\rm ex} = -\frac{3}{4}\,J\,\rho(0), \qquad \rho(0) \equiv \sum_{kk'} \phi_k^*\phi_{k'}\,\psi_k^*(\mathbf{0})\psi_{k'}(\mathbf{0}) = \sum_k |\phi_k|^2 \;=\; 1.$$

(The last step uses plane waves $\psi_k(\mathbf{0}) = 1/\sqrt{V}$ and the normalisation of ϕ_k.)

$$\boxed{E[\phi] = \sum_{\epsilon_k>0} |\phi_k|^2\epsilon_k - \frac{3}{4}\,J.}$$

5. Minimisation via Lagrange Multiplier

Minimise $E[\phi] + \lambda\big(\sum_{\epsilon_k>0}|\phi_k|^2 - 1\big)$:

$$\frac{\partial}{\partial\phi_k^*}\Big[|\phi_k|^2\epsilon_k + \lambda|\phi_k|^2\Big] = 0 \quad\Longrightarrow\quad (\epsilon_k-\lambda)\,\phi_k = 0 \;\;+\;\text{constraint}\;\sum|\phi_k|^2 = 1.$$

Non-trivial solution:

$$\phi_k = \frac{A}{\epsilon_k-\lambda}, \qquad A \text{ fixed by norm.}$$

Self-Consistency Equation

Insert ϕ_k into normalisation:

$$1 = |A|^2\sum_{\epsilon_k>0}\frac{1}{(\epsilon_k-\lambda)^2} \quad\xrightarrow[\text{flat band}]{}\quad |A|^2\rho_0\int_0^D\frac{\mathrm{d}\epsilon}{(\epsilon-\lambda)^2},$$

and into kinetic energy:

$$\sum_{\epsilon_k>0}\frac{|\phi_k|^2\,\epsilon_k}{1} \;=\; |A|^2\rho_0\int_0^D\frac{\epsilon\,\mathrm{d}\epsilon}{(\epsilon-\lambda)^2}.$$

After evaluating both integrals, normalising and substituting into $E[\phi]$, one finds

$$E_{\rm var}(\lambda) = \lambda - \frac{3}{4}\,J, \qquad \text{with constraint}\;\; 1 = \frac{3}{4}\,J\rho_0\ln\frac{D-\lambda}{-\lambda}.$$

Solution for λ

Because $J>0$ and $\rho_0 J \ll 1$, the minimal solution has $\lambda<0,\ |\lambda| \ll D$:

$$\boxed{|\lambda| = D\exp\big[-4/(3J\rho_0)\big] \;\equiv\; k_B T_K.}$$

Hence

$$\boxed{E_{\rm bind} = -k_B T_K - \frac{3}{4}\,J \approx -k_B T_K, \qquad T_K = De^{-1/(J\rho_0)} \text{ (up to a prefactor).}}$$

6. Real-Space Form of the Screening Cloud

Fourier transforming the optimal ϕ_k:

$$\phi_k \propto \frac{1}{\epsilon_k + |\lambda|} \quad\Longrightarrow\quad \phi(r=|\boldsymbol{r}|) \;\propto\; \frac{\sin k_F r}{k_F r}\, e^{-r/\xi_K}, \quad \xi_K = \frac{\hbar v_F}{\pi k_B T_K}.$$

* ξ_K is the "Kondo screening length" (hundreds nm in metals). * The impurity spin is screened by an extended cloud of conduction electrons whose density decays on scale ξ_K.

7. Physical Picture

- Variational optimisation trades *kinetic cost* (broad momentum distribution) against *exchange gain.*
- The result is an exponentially small binding energy that matches the exact Kondo scale up to order-one prefactors.
- Unlike the large-N mean-field method, the Yosida/Varma–Yafet ansatz retains explicit SU(2) symmetry and yields a *true singlet* with binding $-k_B T_K$.

8. Physical Interpretation of the Variational Result

(i) Emergent energy scale. The minimisation produces

$$k_B T_K \;=\; D\exp\big[-\tfrac{1}{J\rho_0}\big] \quad \text{(up to prefactors).}$$

No small parameter in the bare Hamiltonian equals T_K; it is a **non-perturbative** scale generated by the competition between band kinetic energy and antiferromagnetic exchange. Any observable sensitive to the impurity crosses over near $T \sim T_K$.

(ii) Binding energy and singlet formation. The variational ground-state energy

$$E_{\text{var}} \simeq -k_B T_K$$

is **negative and exponentially small**. It represents the energy gained when the impurity spin locks into a *singlet* with the conduction band:

$$\boxed{|\Psi_{\text{gs}}\rangle \approx \frac{1}{\sqrt{2}}\Big(|\Uparrow\rangle_{\text{imp}} |\Downarrow\rangle_{\text{cloud}} - |\Downarrow\rangle_{\text{imp}} |\Uparrow\rangle_{\text{cloud}}\Big).}$$

At $T=0$ the impurity's free-spin entropy $\ln 2$ is thus quenched.

(iii) Kondo screening cloud. Fourier transforming the optimal orbital $\phi_k \propto (\epsilon_k + k_B T_K)^{-1}$ gives the real-space envelope

$$|\phi(r)|^2 \propto \frac{\sin^2(k_F r)}{(k_F r)^2} e^{-2r/\xi_K}, \qquad \xi_K = \frac{\hbar v_F}{\pi k_B T_K}.$$

Hence the impurity spin is screened by a diffuse electron cloud that extends over hundreds of lattice spacings in typical metals. Detecting this "**Kondo cloud**"—the spatial footprint of many-body entanglement—is an ongoing experimental challenge.

(iv) Low-temperature Fermi-liquid behaviour. Because the screened singlet is non-degenerate, low-energy excitations must be *elastic* scattering of conduction electrons from a potential that preserves spin. This corresponds to the **unitary-limit** phase shift $\delta(\omega = 0) = \pi/2$, reproducing the $T \to 0$ Fermi-liquid picture of Nozières.

(v) Limitations of the ansatz. The single-electron dressing captures the exponential scale correctly, but it *omits* multi-electron particle-hole excitations that become important for quantitative thermodynamics ($C(T)$, $\chi(T)$). Full NRG or Bethe ansatz treatments systematically include those states.

Together, items (i)–(v) show that even a "minimal" Yosida/Varma–Yafet trial state already encodes the essential Kondo physics: an exponentially small binding scale, formation of a many-body singlet, a spatial screening cloud, and the onset of Fermi-liquid behaviour at low temperature.