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► **To cite this version:**

H. Kaga, K. Yosida. ANDERSON ORTHOGONALITY DUE TO LOCAL ELECTRON CORRELATION. Journal de Physique Colloques, 1978, 39 (C6), pp.C6-846-C6-847. 10.1051/jphyscol:19786376 . jpa-00217843

HAL Id: jpa-00217843

<https://hal.science/jpa-00217843>

Submitted on 4 Feb 2008

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ANDERSON ORTHOGONALITY DUE TO LOCAL ELECTRON CORRELATION

H. Kaga^{†*} and K. Yosida^{**}

† Department of Physics, Niigata University, Niigata 950-21, Japan

Résumé.- On montre que la catastrophe d'orthogonalité due à la corrélation électronique locale U apparaît dans le modèle asymétrique d'Anderson, mais pas dans le modèle symétrique.

Abstract.- The orthogonality catastrophe due to the local electron correlation U is shown to exist in the asymmetric but not symmetric Anderson model

Does the Anderson orthogonality catastrophe /1/ arise in the presence of local electron-electron interaction? If it does, what is responsible for it, its local character or the localization of charge (or spin)? We show that the orthogonality catastrophe results only in the asymmetric case but not in the symmetric case of the Anderson model, and that the many-body orthogonality index can also be expressed in terms of change in local (d-) electron number /2/.

Separating out the mean-field Coulomb potential $U\langle n_d \rangle a_{d\sigma}^+ a_{d\sigma}$ from perturbation the general asymmetric Anderson model is written :

$$H_0 = \sum_{k\sigma} \epsilon_k a_{k\sigma}^+ a_{k\sigma} + V \sum_k (a_{k\sigma}^+ a_{d\sigma} + a_{d\sigma}^+ a_{k\sigma}) + \epsilon_d \sum_{\sigma} a_{d\sigma}^+ a_{d\sigma} - U\langle n_d \rangle^2 \tag{1}$$

$$H' = U(n_{d\uparrow} - \langle n_{d\uparrow} \rangle)(n_{d\downarrow} - \langle n_{d\downarrow} \rangle) \tag{2}$$

where $\epsilon_d = \epsilon_d^0 + U\langle n_d \rangle$, ϵ_d^0 is the d-level in the absence of U and $\langle n_d \rangle$ the number of d-electrons in the absence of H'. We study the overlap integral between the two ground states, $|\Psi_0\rangle \equiv |0\rangle$ without and $|\Psi\rangle \equiv |>$ with H', by a perturbation method :

$$\langle \Psi_0 | \Psi \rangle = \lim_{t \rightarrow \infty} \langle \Psi_0 | S(t) | \Psi_0 \rangle = \lim_{t \rightarrow \infty} \exp[\overline{C}(t)] \tag{3}$$

Here $C(t) \equiv \langle S(t) \rangle_{0,c}$ is the connected part of the S-matrix.

In order to investigate the possibility of the orthogonality catastrophe we are interested, among various connected terms in each order in C(t)

[†] Permanent address
^{*} Present address : Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801 USA
^{**} The Institute for Solid State Physics, The University of Tokyo, Japan

only in the divergent ones for $t \rightarrow \infty$, which turn out to be at most logarithmic. Detailed examination tells us that logarithmic divergence appears as $(\ln t)$ only in some particular connected diagrams of fourth and higher orders ; second- and third-order connected diagrams give no divergence. Figure 1 shows the two typical examples (a), (b) of such renormalized diagrams in time-representation, in which both vertex and self-energy corrections are assumed to have been made.

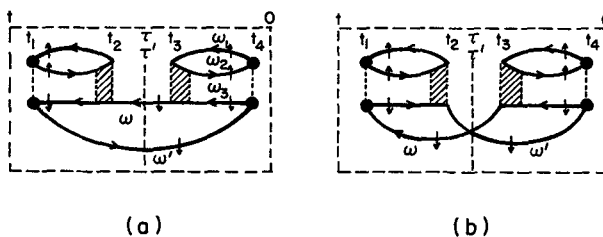


Fig. 1 : The two basic renormalized divergent connected diagrams (a),(b). The halves divided by dotted lines are the diagrams that give the dominant contributions for change in the localized d-electron number.

These two divergent contributions $C_a(t)$ and $C_b(t)$ are :

$$C_a(t) = (\tilde{U}\tilde{U})^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \int_0^{t_3} dt_4 [-G_{12}^0 G_{23}^0 G_{34}^0 G_{41}^0] + \left[\frac{\tilde{U}\tilde{U}\Delta}{\pi(\Delta^2 + \epsilon_d^2)} \right]^2 \{\alpha^>\}^2 \ln t \tag{4}$$

$$C_b(t) \sim \left[\frac{\tilde{U}\tilde{U}\Delta}{\pi(\Delta^2 + \epsilon_d^2)} \right]^2 \{\alpha^>\alpha^<\} \ln t \tag{5}$$

where $G_{ij}^0 \equiv G^0(t_i - t_j)$ $\alpha^> \equiv \alpha^>(0)$

$$G^0(t) = \frac{1}{\pi} \int_{0,(-\infty)}^{\infty, (0)} g^0(\omega) e^{-i\omega t} d\omega, t > 0 (t < 0) \tag{6}$$

$$\alpha^>(\omega) = \frac{1}{\pi^3} \int_0^\infty d\omega_1 d\omega_3 \int_{-\infty}^0 d\omega_2 \frac{g^0(\omega_1) g^0(\pm\omega_3) g^0(\omega_2)}{\omega_1 + \omega_3 - \omega_2 \pm \omega} \quad (7)$$

$$g^0(\omega) = \frac{-i\Delta \operatorname{sgn}\omega}{(\omega - \epsilon_d)^2 + \Delta^2} \quad (8)$$

$\Delta = \pi\rho v^2$, ρ is the density of s -electron states at the Fermi energy ϵ_F , from which all energies are measured. There are two other divergent diagrams (c), (d) (not shown) obtained by reversing the electron-lines (\leftarrow) to the holes-lines (\rightarrow) and vice-versa for down-spin (\downarrow) in figure 1 (a) and (b) and four diagrams constructed by interchanging up (\uparrow) and down-spins (\downarrow) in (a) \sim (d). Putting together the total divergent contribution $C(t)$ amounts to :

$$C(t) = 2 \left\{ \frac{U\tilde{U}\Delta}{\pi(\Delta^2 + \epsilon_d^2)} \right\}^2 \{\alpha^> + \alpha^<\}^2 \ln t$$

$$= -2\{\gamma(U, \epsilon_d)\}^2 \ln t \quad (9)$$

$$\gamma(U, \epsilon_d) = \frac{U\tilde{U}}{\Delta^2} \cdot \frac{\epsilon_d}{\Delta^2 + \epsilon_d^2} \left\{ \left[\frac{2}{\pi} \right]^2 \int_0^\infty d\omega_1 d\omega_3 \int_{-\infty}^0 d\omega_2 \right.$$

$$\left. \times \frac{\omega_3 g^0(\omega_1) g^0(\omega_3) g^0(-\omega_3) g^0(\omega_2)}{\omega_1 + \omega_3 - \omega_2} \right\}, \quad (10)$$

which becomes an effective interaction constant of real dimensionless quantity except the sign. Equations (3), (9) and (10) demonstrate the following results. (i) In the general asymmetric case, where $\gamma(U, \epsilon_d) \neq 0$, the ground state overlap $\langle S(t) \rangle_0$ vanishes for $t \rightarrow \infty$; (ii) in the case of the so-called electron-hole symmetry, $\epsilon_d = \epsilon_d^0 + U/2 = 0$ where $\epsilon_d^0 = 0$ for $U = 0$ and $\epsilon_d = \epsilon_d^0 + U/2 = 0$ for $U \neq 0$ we have $\gamma(U, 0) = 0$ and thus no orthogonality catastrophe exists.

We calculate change in the d -electron localization due to H' , $\delta n = \langle n_d \rangle - \langle n_d \rangle_0$:

$$\delta n = \lim_{\tau' \rightarrow \tau + 0} -i [\bar{G}(\tau, \tau') - G^0(\tau, \tau')]$$

$$= \lim_{\tau' \rightarrow \tau + 0} (-iUU) \int_{-\infty}^\infty dt_1 \int_{-\infty}^{\tau_1} dt_2 [\bar{G}_{\tau_1 12}^0 G_{12}^0 G_{2\tau'}^0 + G_{\tau_2 21}^0 G_{21}^0 G_{1\tau}^0]$$

$$[\bar{G}_{12}^0 G_{21}^0] \quad (11)$$

We notice in figure 1 that the diagrams for the two terms of $\delta \tilde{n}^{(2)}$ correspond exactly to the halves of the diagrams $C_a(t)$ and $C_b(t)$ if we put τ, τ' on the central dotted lines; in fact, the diagrams of $\delta \tilde{n}^{(2)}$ all appear in the $C(t)$ diagrams. We obtain

$$\delta \tilde{n}^{(2)} = \left[\frac{iU\tilde{U}}{\pi(\Delta^2 + \epsilon_d^2)} \right] \{\alpha^> + \alpha^<\}$$

$$= \gamma(U, \epsilon_d) \quad (12)$$

According as whether $\epsilon_d > 0$ or $\epsilon_d < 0$, we have $\delta \tilde{n}^{(2)} > 0$ or $\delta \tilde{n}^{(2)} < 0$; thus the effective coupling constant is given by $-\gamma(U, \epsilon_d)$ and this is attractive for $\epsilon_d > 0$ and repulsive for $\epsilon_d < 0$, which is physically natural. From eqs. (9) and (12)

$$C(t) = -2\{\delta \tilde{n}^{(2)}\}^2 \ln t \quad (13)$$

We expect that the Anderson orthogonality catastrophe holds quite generally for any local perturbation of electron-electron interaction as well as one-electron scattering potential when the change of local charge is accompanied.

References

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