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LETTER TO THE EDITOR

The Anderson model in a superconductor: Φ-derivable theory

Ari T Alastalo†, Robert J Joynt‡ and Martti M Salomaa†‡

† Materials Physics Laboratory, PO Box 2200 (Technical Physics), Helsinki University of Technology, FIN-02015 HUT, Finland

‡ Department of Physics and Applied Superconductivity Center, University of Wisconsin–Madison, Madison, WI 53706, USA

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Abstract. We introduce a new Φ-derivable approach for the Anderson impurity model in a BCS superconductor. The regime of validity of this conserving theory extends well beyond that of the Hartree–Fock approximation. This is the first generalization of the U-perturbation theory to encompass a superconductor.

The Anderson impurity model [1] provides one of the most versatile field-theoretic descriptions for interacting correlated electrons within condensed-matter physics [2]. The Anderson Hamiltonian in a normal metal is

$$\mathcal{H}_A = \mathcal{H}_s + \mathcal{H}_{sd} + \mathcal{H}_d + \mathcal{H}_U \tag{1}$$

where $\mathcal{H}_s = \sum_{k,\sigma} \varepsilon_{k\sigma} n_{k\sigma}$ describes the electron gas, $\mathcal{H}_{sd} = \sum_{k,\sigma} (V_k c^\dagger_{k\sigma} d_\sigma + V^*_k d^\dagger_\sigma c_{k\sigma})$ is the admixture interaction, $\mathcal{H}_d = \sum_\sigma E_\sigma n_\sigma$ represents the d-electron level and $\mathcal{H}_U = U n_\uparrow n_\downarrow$ denotes the Coulomb-repulsion interaction. This model describes the continuous transition of a nonmagnetic resonant level (for $U \ll \Gamma$, where $\Gamma = \pi N(0)\langle |V|^2 \rangle$) to a magnetic atom ($U \gg \Gamma$), and one can consider treating either V or U perturbatively. For $\Gamma/U \ll 1$, in the magnetic Schrieffer–Wolff (SW) limit [3], the Anderson Hamiltonian reduces to the s–d Hamiltonian, i.e. the Kondo model. This limit and the magnetic–nonmagnetic transition have been successfully treated within the renormalization group (RNG) program [4]. However, simpler controlled approaches would be highly desirable due to the wide applicability of the Anderson model and its variants to many physical systems of interest.

Since its initial introduction to describe the nonmagnetic–magnetic transition of impurities in otherwise nonmagnetic metals, and the associated many-body Kondo phenomenology, the Anderson model has been extensively applied and generalized to also describe interacting pairs of impurity atoms in metals (the Alexander–Anderson model), valence fluctuations and heavy-fermion materials (the periodic Anderson model), chemisorption (the Anderson–Newns model) and charging phenomena and the Coulomb blockade in quantum dots and quantum-dot arrays. It is also of great inherent interest to consider the Anderson model for a superconductor and the appropriate theoretical approaches to this problem. In particular, the RNG approach has not been generalized to this case and the Bethe-*ansatz* (BA) method fails to be suitable since the superconducting electronic spectrum does not fulfil the requirement of a linear ($\varepsilon_k \propto k$) dispersion relationship, necessary for the applicability of the k-state enumeration within the BA scheme.

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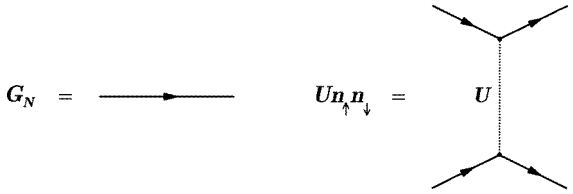

Figure 1. The local d-electron propagator in the normal state, $G_N(\omega)$, is here denoted as a line with an arrowhead (l.h.s.). The local Coulomb-repulsion or Anderson–Hubbard-interaction term $Un_\uparrow n_\downarrow$ is represented in the diagrams with a dashed line having two vertices (r.h.s.).

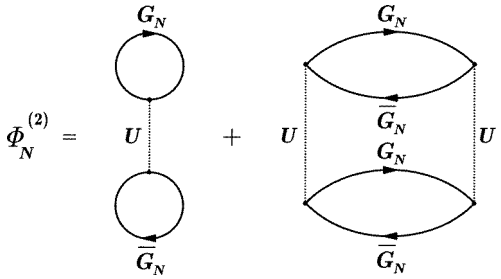

Figure 2. The terms $\Phi_N^{(2)}$ in the normal state up to the second order in U. The linear term in U is the Hartree–Fock bubble. The second-order term in U contains two particle–hole (susceptibility) bubbles, describing interacting localized spin fluctuations (LSF) at the impurity site.

Yosida and Yamada [5] first pointed out that in order to obtain the single-particle Green's function and the local density of impurity d states, it is useful to study the many-body perturbation theory with respect to U. Thus one considers the Anderson Hamiltonian as

$$\mathcal{H}_A = \mathcal{H}^0_{HF} - U\langle n_\uparrow\rangle\langle n_\downarrow\rangle + \mathcal{H}'_U \tag{2}$$

where $\mathcal{H}^0_{HF} - U\langle n_\uparrow\rangle\langle n_\downarrow\rangle$ is up to the constant energy shift, $U\langle n_\uparrow\rangle\langle n_\downarrow\rangle$, the unperturbed Hartree–Fock (HF) Hamiltonian and

$$\mathcal{H}'_U = U\,\delta n_\uparrow\,\delta n_\downarrow = U(n_\uparrow - \langle n_\uparrow\rangle)(n_\downarrow - \langle n_\downarrow\rangle) \tag{3}$$

is the Coulomb-repulsion term, treated as the perturbation; see figure 1. Yosida and Yamada, in their original paper [5], used a complicated formalism utilizing Pfaffian determinants to derive the U-perturbation theory; Yamada [6] first presented the numerically evaluated d-electron spectral density function using the U^2-self-energy in the low-temperature limit. This approach may easily be generalized to arbitrary temperatures in normal metals [7], for which one may introduce the d-electron impurity self-energy $\Sigma_N(\omega)$ through

$$G_N(\omega) = \Big((G_{HF})^{-1} - \Sigma_N(\omega)\Big)^{-1}. \tag{4}$$

Here the HF propagator is

$$G_{HF}(\omega) = -\Big(\omega - E_{HF} - F(\omega)\Big)^{-1} \tag{5}$$

with $F(\omega) = \sum_k |V_k|^2 G^0_k(\omega) \approx -\mathrm{i}\Gamma$ and $G^0_k(\omega) = (\omega - \varepsilon_k)^{-1}$. Above, $E_{HF} = U + \langle n\rangle$ is the Hartree–Fock energy. Here and in what follows we omit the spin indices for brevity; hence our expressions are valid for zero field. Using the second-order free-energy functional

$\Phi_N^{(2)}$ in figure 2, one easily finds that the U^2-self-energy may be obtained by cutting the d-electron propagator line in the diagram as

$$\Sigma_N = \delta\Phi_N/\delta G_N. \tag{6}$$

Consequently, the imaginary part of the second-order contribution (in U) to the impurity self-energy is given by

$$\Sigma_N''(\omega) = U^2 \int \frac{\mathrm{d}\omega_1}{\pi} \int \frac{\mathrm{d}\omega_2}{\pi} \int \mathrm{d}\omega_3 \; \delta(\omega - \omega_1 - \omega_2 - \omega_3) F(\omega_1, \omega_2, \omega_3) G_{HF}''(\omega_1) \times G_{HF}''(\omega_2) G_{HF}''(\omega_3). \tag{7}$$

Here $F(\omega_1, \omega_2, \omega_3)$ abbreviates the following collection of thermal occupancy factors:

$$F(\omega_1, \omega_2, \omega_3) = [1 - f(\omega_1)][1 - f(\omega_2)][1 - f(\omega_3)] + f(\omega_1) f(\omega_2) f(\omega_3) \tag{8}$$

with $f(\omega) = (\mathrm{e}^{\omega/T} + 1)^{-1}$ denoting the Fermi distribution function.

Note that the U-perturbation theory can be derived from a free-energy functional, Φ. Therefore, this is a 'conserving approximation' [8] for the many-body system, with positive definite spectral functions and with sum rules fulfilled by construction. The linear term in U—see figure 2—is the HF term, describing the motion of a d electron with spin σ in the mean field produced by the d electron with spin $-\sigma$. This mean field, or the expectation value $\langle n \rangle$, must be computed self-consistently. The quadratic term in U describes the interaction, at the impurity site, of the localized spin fluctuations (LSF) represented by the particle–hole spin-susceptibility bubbles ($G_N \bar{G}_N$).

Yamada [6] first showed that the U^2-self-energy $\Sigma_N^{(2)}(\omega)$ yields a triple-peaked structure for the spectral density of the impurity atom. The sharp central peak for $T = 0$ obtains the unitary limiting value at $\omega = 0$. This approach was later generalized to arbitrary finite temperatures [7] and it was shown that the central zero-frequency peak has a sensitive T-dependence.

The Anderson model in a superconductor is given by

$$\mathcal{H}_{A,BCS} = \mathcal{H}_{BCS} + \mathcal{H}_{sd} + \mathcal{H}_d + \mathcal{H}_U \tag{9}$$

where the BCS Hamiltonian is

$$\mathcal{H}_{BSC} = \sum_{k,\sigma} \varepsilon_{k\sigma} n_{k\sigma} - \sum_k (\Delta c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \Delta^* c_{-k\downarrow} c_{k\uparrow}). \tag{10}$$

This model has been discussed in the HF [9, 10] and Schrieffer–Wolff [11] limits. In the HF approximation for a superconductor one truncates the Coulomb-interaction term as follows:

$$U n_\uparrow n_\downarrow \to U\langle n_\uparrow \rangle n_\downarrow + U\langle n_\downarrow \rangle n_\uparrow + U\langle d_\uparrow^\dagger d_\downarrow^\dagger \rangle d_\downarrow d_\uparrow + U\langle d_\downarrow d_\uparrow \rangle d_\uparrow^\dagger d_\downarrow^\dagger. \tag{11}$$

Here the anomalous average $\langle d_\downarrow d_\uparrow \rangle$ induced at the impurity site presents another mean field, in addition to $\langle n \rangle$, which is to be computed self-consistently. The HF approximation to the Anderson model in a superconductor [9] shares the same instability problem as the HF approximation in the normal metal [1]: a spontaneous unphysical breaking of symmetry at the impurity site. Our aim is to develop an approach which is free from this HF instability and which enables one to go beyond the HF picture. In particular, we are interested in investigating the qualitatively new physical features, especially in the d-electron density of states, due to increasing electron correlations as U increases beyond $\pi\Gamma$, where the HF solution no longer provides quantitatively meaningful answers.

A generalization of the U-perturbation theory for the Anderson model in a superconductor has thus far not been discussed in the literature. The purpose of this letter is to suggest a new, conserving, self-energy U-perturbation expansion that is valid in a

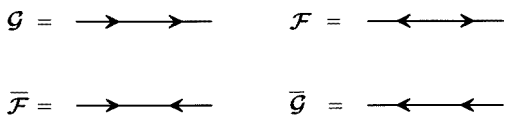

Figure 3. Elements of the localized 2×2 Green's-function matrix in the Nambu space for the superconducting state are represented by lines with double arrows. Here $\mathcal{G}(\omega)$, corresponding to the $G_N(\omega)$ in figure 1, is the electron propagator, while $\bar{\mathcal{G}}(\omega)$ is the time-reversed hole-propagator function; $\mathcal{F}(\omega)$ is the anomalous particle–hole Green's function and $\bar{\mathcal{F}}(\omega)$ denotes its conjugate.

superconductor. We note that the RNG approach has recently been generalized to treat magnetic impurities in superconductors, but thus far only for the s–d model [12].

The matrix self-energy expansion in the Nambu space is introduced as

$$\hat{G}_S(\omega) = \left((\hat{G}_{HF}(\omega))^{-1} - \hat{\Sigma}_S(\omega) \right)^{-1} \tag{12}$$

where the hat denotes matrices in the particle–hole Nambu space and the d-electron propagator in the HF approximation is given as

$$\hat{G}_{HF}(\omega) = -\begin{pmatrix} \omega - E_{HF} - F_{11}(\omega) & U\langle d_\sigma d_{-\sigma}\rangle - F_{12}(\omega) \\ U\langle d^\dagger_{-\sigma} d^\dagger_\sigma\rangle - F_{21}(\omega) & \omega + E_{HF} - F_{22}(\omega) \end{pmatrix}^{-1} \tag{13}$$

which, for brevity, we denote here as

$$\hat{G}_{HF}(\omega) = \begin{pmatrix} \mathcal{G}(\omega) & \mathcal{F}(\omega) \\ \bar{\mathcal{F}}(\omega) & \bar{\mathcal{G}}(\omega) \end{pmatrix}. \tag{14}$$

These propagators are illustrated graphically in figure 3 as lines with two arrows.

The energy-integrated Green's function (or generalized density of states) $\hat{F}_S(\omega)$ in equation (13) is

$$\hat{F}_S(\omega) = \begin{pmatrix} F_{11}(\omega) & F_{12}(\omega) \\ F_{21}(\omega) & F_{22}(\omega) \end{pmatrix} = \sum_k \hat{V}_k^* \hat{G}_k^0(\omega) \hat{V}_k \tag{15}$$

where

$$\hat{V}_k = \begin{pmatrix} V_k & 0 \\ 0 & -V_k^* \end{pmatrix}. \tag{16}$$

Above, in equation (15), $\hat{G}_k^0(\omega)$ is the unperturbed Green's function for the bulk superconductor:

$$\hat{G}_k^0(\omega) = \begin{pmatrix} \omega - \varepsilon_k & \Delta \\ \Delta^* & \omega + \varepsilon_{-k} \end{pmatrix}^{-1}. \tag{17}$$

The self-energy in equation (12) is a matrix in the Nambu space:

$$\hat{\Sigma}_S(\omega) = \begin{pmatrix} \Sigma_{11}(\omega) & \Sigma_{12}(\omega) \\ \Sigma_{21}(\omega) & \Sigma_{22}(\omega) \end{pmatrix} \tag{18}$$

which may be obtained as

$$\Sigma_{ij} = \delta\Phi_S / \delta(G_S)_{ij} \tag{19}$$

where Φ_S now denotes the free energy in a superconductor.

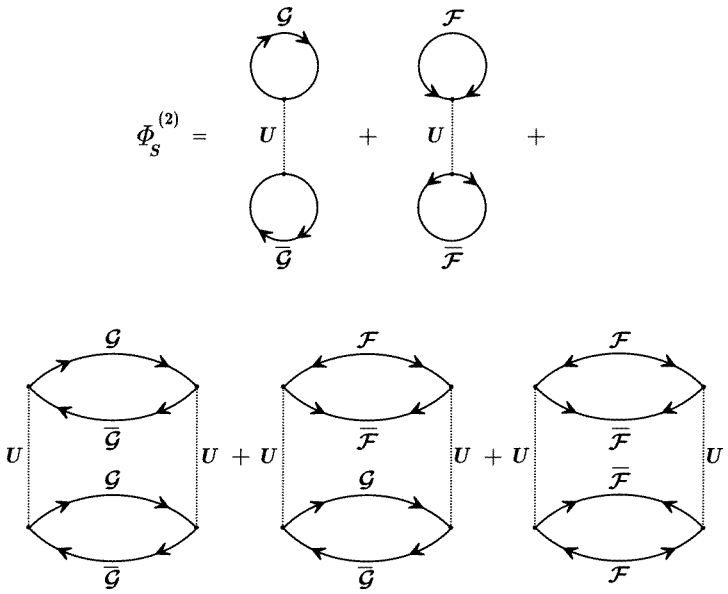

Figure 4. The generalization of Φ to the second order in U for the pair-correlated state, $\Phi_S^{(2)}$, expressed in terms of the superconducting propagators, $\mathcal{G}$, $\bar{\mathcal{G}}$, $\mathcal{F}$ and $\bar{\mathcal{F}}$, in figure 3. Due to the anomalous propagators in the pair-correlated medium, there now occur two first-order Hartree–Fock terms linear in U and three second-order terms in U, owing to the interacting localized spin fluctuations (LSF), correlated localized spin and pairing fluctuations (LSPF) and interacting localized pairing fluctuations (LPF), respectively.

The second-order free-energy term in U for a superconductor, $\Phi_S^{(2)}$, is illustrated in figure 4 from which we obtain the following expression, accurate to U^2:

$$\begin{pmatrix} \Sigma''_{11}(\omega) & \Sigma''_{12}(\omega) \\ \Sigma''_{21}(\omega) & \Sigma''_{22}(\omega) \end{pmatrix} = U^2 \int \frac{\mathrm{d}\omega_1}{\pi} \int \frac{\mathrm{d}\omega_2}{\pi} \int \mathrm{d}\omega_3 \; \delta(\omega - \omega_1 - \omega_2 - \omega_3) F(\omega_1, \omega_2, \omega_3) \times \begin{pmatrix} \mathcal{G}''(\omega_1) & -\mathcal{F}''(\omega_1) \\ -\bar{\mathcal{F}}''(\omega_1) & \bar{\mathcal{G}}''(\omega_1) \end{pmatrix} \left(\mathcal{G}''(\omega_2)\bar{\mathcal{G}}''(\omega_3) - \mathcal{F}''(\omega_2)\bar{\mathcal{F}}''(\omega_3) \right) \tag{20}$$

where $F(\omega_1, \omega_2, \omega_3)$ is, again, given by equation (8). Note that the propagators $\mathcal{G}$, $\bar{\mathcal{G}}$, $\mathcal{F}$ and $\bar{\mathcal{F}}$ in the above expression may be evaluated in the HF approximation—see equation (13)—which already contains the pairing interaction $\mathcal{H}_{BCS}$ to infinite order in the unperturbed Hamiltonian $\mathcal{H}^0$. Therefore, the ω-integrals in equation (20) are rather complicated: they contain delta-function contributions from the bound states and also continuum contributions. Trivially, one observes that the normal-state limit, equation (7), is obtained consistently from equation (20) when $\Delta \to 0$ and that the diagrams in figure 4 reduce to those in figure 2 for $\Delta \to 0$.

The free-energy diagrams in figure 4 now comprise two contributions linear in U, corresponding to the self-consistent occupation-number field $\langle n \rangle$, and the induced anomalous average (the proximity pairing at the impurity d-orbital site) $\langle d_\downarrow d_\uparrow \rangle$. Furthermore, there now occur three terms quadratic in U. Two of these terms are due to the localized spin fluctuations (LSF), represented by the spin-susceptibility bubble ($\mathcal{G}\bar{\mathcal{G}}$), mutually interacting at the impurity site and also with the induced localized pairing fluctuations (LPF), shown as the pairing-susceptibility bubble ($\mathcal{F}\bar{\mathcal{F}}$). The third contribution arises from the induced mutually interacting localized pairing fluctuations.

Preliminary numerical results [13] indicate the doubling of bound states, in comparison to the HF theory. In particular, the new bound states tend towards $\omega = 0$ for increasing U. We shall discuss the full numerical results in detail elsewhere. Our approach can also be readily extended to other situations of interest, such as an Anderson impurity in unconventional superconductors [14]. In this case, the self-energy expressions are formally the same but the order parameter must in general be interpreted as a matrix in spin space. Also the order parameter $\Delta(\hat{k})$ for unconventional superconductors possesses less rotational symmetry than that in the s-wave case. This will naturally lead to a $\hat{k}$-dependence of the d-electron Green's function $\hat{G}_S(\hat{k}, \omega)$, the matrix self-energy $\hat{\Sigma}_S(\hat{k}, \omega)$ and the bound-state spectrum below the $\hat{k}$-dependent energy-gap edge.

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References

[1] Anderson P W 1961 *Phys. Rev.* **124** 41
[2] Hewson A C 1993 *The Kondo Problem and Heavy Fermions* (Cambridge: Cambridge University Press)
[3] Schrieffer J R and Wolff P A 1966 *Phys. Rev.* **149** 491
[4] Krishna-murthy H R 1978 *PhD Thesis* Cornell University
Krishna-murthy H R, Wilkins J W and Wilson K G 1980 *Phys. Rev.* B **21** 1003
Krishna-murthy H R, Wilkins J W and Wilson K G 1980 *Phys. Rev.* B **21** 1044
[5] Yosida K and Yamada K 1970 *Prog. Theor. Phys. Suppl.* **46** 244
[6] Yamada K 1975 *Prog. Theor. Phys.* **53** 970
[7] Salomaa M M 1981 *Solid State Commun.* **38** 1105
Salomaa M M 1981 *Solid State Commun.* **39** 1195
[8] Baym G and Kadanoff L P 1961 *Phys. Rev.* **124** 287
Baym G 1962 *Phys. Rev.* **127** 1391
[9] Shiba H 1972 *Solid State Commun.* **11** 1735
Shiba H 1973 *Prog. Theor. Phys.* **50** 50
[10] Kim H and Muzikar P 1993 *Phys. Rev.* B **48** 3933
[11] Salomaa M M 1988 *Phys. Rev.* B **37** 9312
[12] Satori K, Shiba H, Sakai O and Shimizu Y 1992 *J. Phys. Soc. Japan* **61** 3239
Sakai O, Shimizu Y, Shiba H and Satori K 1993 *J. Phys. Soc. Japan* **62** 3181
Shiba H 1995 *Computational Physics as a New Frontier in Condensed Matter Research* (Tokyo: The Physical Society of Japan) p 156
[13] Alastalo A T and Salomaa M M 1997 *9th Int. Conf. on Recent Progress in Many-Body Theories (Sydney, 1997)*
[14] Joynt R J 1998 *J. Low Temp. Phys.* at press