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A Rigorously Solvable Model of a Magnetic Ion in a Superconductor

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Abstract. A magnetic ion, described by the Anderson Hamiltonian is coupled to a strong coupling superconductor (kinetic energy is neglected). Exact conditions for the magnetic state are derived.

Only a very small number of many body problems are solvable. An exactly solvable model of a superconductor (the 'strong coupling superconductor') has been proposed by Wada [1] and Anderson [2]. This is a very unrealistic model, but its solution displays some of the simpler properties of a superconductor.

In this note we consider a magnetic impurity, described by the Anderson Hamiltonian, which interacts with a strong coupling superconductor. We find the exact solution of the groundstate and derive the condition for the occurence of a magnetic moment. Again the model is very unrealistic, but it demonstrates how the local magnetic state is incorporated into a many body state of the whole system.

For a single magnetic ion which is coupled to a large system only through the chemical potential (electron reservoir), the Anderson Hamiltonian [3] reads

$$H_0 = -E\,(n_{0\uparrow} + n_{0\downarrow}) + U\, n_{0\uparrow}\, n_{0\downarrow}\,. \tag{1}$$

Here $-E$ is the unperturbed energy of the magnetic ion, and U is the Coulomb repulsive energy between electrons in the states $|0\uparrow\rangle$ and $|0\downarrow\rangle$. For convenience the chemical potential μ is included in E. The ground state of (1) is nonmagnetic if the energy $-2\,E + U$ of the doubly occupied state is lower than $-E$. Thus the condition for a magnetic behavior is simply

$$U > E\,. \tag{2}$$

In the strong-coupling limit (where the kinetic energy is neglected) the superconductivity problem can be solved exactly [3]. In this limit we can easily transform the BCS Hamiltonian into the Wannier representation, so that

$$H = -\frac{V}{N} \sum_{i,j} c_{i\uparrow}^+ c_{i\downarrow}^+ c_{j\downarrow} c_{j\uparrow} . \tag{3}$$

N is the number of atoms.

Let us introduce the spin operators

$$S_i^+ = c_{i\downarrow} c_{i\uparrow} , \tag{4}$$

$$S_i^- = c_{i\uparrow}^+ c_{i\downarrow}^+ , \qquad S_i^z = \frac{1}{2} (1 - n_{i\uparrow} - n_{i\downarrow}) .$$

Then the Hamiltonian (3) becomes

$$H = -\frac{V}{N} S^- S^+ , \tag{5}$$

where $S^\pm = \sum_i S_i^\pm$. Equation (5) has the exact eigenvalues

$$E = -\frac{V}{N} [S (S + 1) - M^2 - M] , \tag{6}$$

where $S = 0, 1/2, \dots , 1/2 (N - 1)$. M has to satisfy the relation

$$n = N - 2 M \tag{7}$$

with n = number of electrons.

In the following we show that the coupled system consisting of the magnetic ion, equation (1), and the superconductor, equation (3), can be solved exactly for the following nontrivial coupling:

$$H_{int} = -\frac{\lambda V}{N} \sum_{i \neq 0} (c_{i\uparrow}^+ c_{i\downarrow}^+ c_{0\downarrow} c_{0\uparrow} + c_{0\uparrow}^+ c_{0\downarrow}^+ c_{i\downarrow} c_{i\uparrow}) , \tag{8}$$

where λ allows the coupling between the magnetic ion and the large system to be smaller than the BCS-coupling in the large system. The total Hamiltonian may now be written as

$$H = -\frac{V}{N} S^- S^+ - \frac{\lambda V}{N} (S^- S_0^+ + S_0^- S^+) + U S_0^- S_0^+ + E (2 S_0^z - 1) , \tag{9}$$

where $S^\pm = \sum_{i \neq 0} S_i^\pm$.

We will now derive exact conditions (in terms of the parameters λ, V, U and E) for the magnetic instability of our model.

The Hilbertspace of the states of our system is the direct sum of the two subspaces corresponding to $S_0 = 0$ and $S_0 = 1/2$ respectively. Therefore we can calculate the two sets of eigenvalues of H separately:

(a) $S_0 = 0$:

$$E^{(0)} = -\frac{V}{N} [S (S + 1) - M^2 - M] - E \tag{10}$$

where $S = 0, 1/2, \dots, 1/2\,(N-1)$. M has to satisfy the relation

$$n = N - 2 \times (M + m) \tag{11}$$

with n = number of electrons and m is the appropriate eigenvalue of S_0^z. For our discussion we set $n = N$, so that (as $m = 0$):

$$E^{(0)} = -\frac{V}{N}\, S\,(S+1) - E \tag{12}$$

(b) $S_0 = 1/2$:

We have

$$\begin{aligned} H\,|M, m\rangle = &-\frac{V}{N}\,[S\,(S+1) - M^2 - M]\,|M, m\rangle \\ &-\frac{\lambda V}{N}\,[(S - M + 1)\,(S + M)]^{1/2}\left[\left(\frac{1}{2} - m\right)\left(\frac{3}{2} + m\right)\right]^{1/2} |M-1, m+1\rangle \\ &-\frac{\lambda V}{N}\,[(S - M)\,(S + M + 1)]^{1/2}\left[\left(\frac{3}{2} - m\right)\left(\frac{1}{2} + m\right)\right]^{1/2} |M+1, m-1\rangle \\ &+ U\left(\frac{1}{2} - m\right)|M, m\rangle + E\,(2\,m - 1)\,|M, m\rangle\,. \end{aligned} \tag{13}$$

From (11) we obtain $M = \pm 1/2$ (since in this case $m = \pm 1/2$ and $n = N$). If we set $M = +1/2$, we have to diagonalize H with respect to the states $|1/2, -1/2\rangle$ and $|-1/2, 1/2\rangle$. This yields

$$\begin{aligned} E^{(1/2)} = &-\frac{V}{N}\left[S\,(S+1) - \frac{1}{4}\right] + \frac{U}{2} - E \\ &\pm \left[\left(\frac{U}{2} - E + \frac{V}{2\,N}\right)^2 + \left(\frac{\lambda V}{N}\right)^2 \times \left(S + \frac{1}{2}\right)^2\right]^{1/2}, \end{aligned} \tag{14}$$

where S takes the same values as above. The lowest energy state of the set (12) is a doubly degenerate magnetic state, whereas the lowest state of the set (14) is a singlet. Thus the condition for the magnetic instability is

$$\Delta = E_0^{(0)} - E_0^{(1/2)} = 0\,. \tag{15}$$

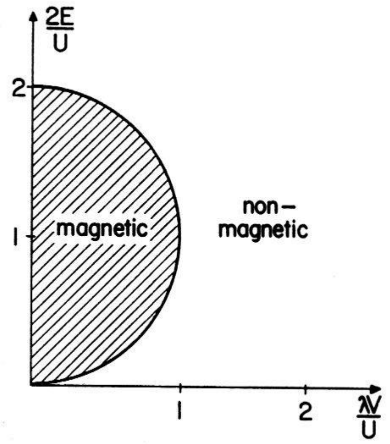
In the limit of large N this gives

$$\Delta = \frac{1}{2}\,\{[(U - 2\,E)^2 + (\lambda\,V)^2]^{1/2} - U\} = 0\,. \tag{16}$$

In terms of the parameters $2\,E/U$ and $\lambda\,V/U$ the boundary between the magnetic and the nonmagnetic region is a half circle (see Figure):

$$\left(\frac{2\,E}{U} - 1\right)^2 + \left(\frac{\lambda\,V}{U}\right)^2 = 1\,. \tag{17}$$

The behavior is quite similar to the case where the magnetic ion is coupled to a free electron gas [3, 4]. In both cases the magnetic state may be suppressed due to the coupling to the large system.



Regions of magnetic and nonmagnetic behavior.

Acknowledgment

This note grew out of a question of Prof. C. Kittel who was concerned with exactly solvable models of superconductivity.

REFERENCES

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[2] P. W. Anderson, Phys. Rev. *112*, 1900 (1958).
[3] For example see: C. Kittel, *Quantum Theory of Solids* (John Wiley & Sons, Inc. 1963), Chapt. 8 resp. Chapt. 18.
[4] For a review see: J. appl. Phys. *39* (1968).