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Geometrical derivation of a new ground state formula for the n-electron Friedel resonance model

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Abstract. The n-electron ground state of the Friedel resonance model can be written as a single Slater determinant of n s-electrons plus *one* d-electron-s-hole companion. This new formula is derived geometrically in the Hilbert space. The derivation uses the fact that a n-electron Slater determinant, built from N band states, corresponds to a n-dimensional subspace in the N-dimensional Hilbert space.

PACS. 71.10.-w Theories and models of many electron systems – 71.55.-i Impurity and defect levels

Recently the author found by numerical variation [1] a new formula for the n-electron ground state of the Friedel Hamiltonian [2]. The Friedel Hamiltonian $\mathrm{H_{Fr}}$ for an s-band with N states and a d resonance has the form:

$$\mathrm{H_{Fr}} = \sum_{\nu=1}^{N} \varepsilon_\nu \mathrm{c}_\nu^* \mathrm{c}_\nu + E_\mathrm{d} d^* d + \sum_{\nu=1}^{N} V_\mathrm{sd}(\nu)[d^* \mathrm{c}_\nu + \mathrm{c}_\nu^* d] \quad (1)$$

where the creation operators c_ν^* describe the N band states with the band energy ϵ_ν and E_d is the energy of the d^* state. (In the following I denote a single electron state by its creation operator and the corresponding vector in Hilbert space by the corresponding bold symbol).

The traditional single electron solutions b_i^* of the Friedel Hamiltonian can be written in the form

$$\begin{aligned} b_i^* &= \beta_i d^* + \sum_{\nu=1}^{N} \beta_{i\nu} c_\nu^* \quad (2)\\ \beta_i &= A_i \\ \beta_{i\nu} &= A_i \frac{V_\nu}{(E_i - \epsilon_n)} \\ A_i &= \frac{1}{\sqrt{1 + \sum_{\nu=1}^{N} \frac{V_\nu^2}{(E_i - \epsilon_\nu)^2}}}. \end{aligned}$$

The energies E_i are the $(N+1)$ eigen energies of the states b_i^* and given by the self consistent relation

$$E_i = E_\mathrm{d} + \sum_{\nu=1}^{N} \frac{|V_\nu|^2}{E_i - \epsilon_\nu}\,. \quad (3)$$

The $(N+1)$ solutions b_i^* of the Friedel Hamiltonian span a $(N+1)$ dimensional Hilbert space. The new basis vectors $\mathbf{b}_i$ are obtained from the N basis vectors $\mathbf{c}_\nu$ plus the $\mathbf{d}$ state by a rotation. The n-electron ground state is represented by the product of the creation operators of the n lowest states (*i.e.* states with the lowest energies)

$$\Psi_0 = \prod_{i=1}^{n} b_i^* \Phi_0. \quad (4)$$

Ψ_0 is a Slater state since it can be written as a single Slater determinant.

The new ground state formula for n electrons which I found numerically can be written in the form of equation (5)

$$\Psi_\mathrm{Fr} = [A a_0^* + B d^*] \prod_{i=1}^{n-1} a_i^* \Phi_0. \quad (5)$$

Here Φ_0 is the vacuum state and a_0^* is localized state which is built from the states of the s-band

$$a_0^* = \sum_{\nu=1}^{N} \alpha_\nu^0 c_\nu. \quad (6)$$

The a_i^* in equation (5) are part of a new orthonormal basis $(a_0^*, a_1^*, ..., a_{N-1}^*)$ for the s-band. The a_i^* $(1 \leq i \leq N-1)$ can be chosen so that their $(N-1)$ sub-matrix of the s-band Hamiltonian $\mathrm{H_0} = \sum \varepsilon_\nu \mathrm{c}_\nu^* \mathrm{c}_\nu$ is diagonal, *i.e.* $\langle a_i \Phi_0 | \mathrm{H_0} | a_j \Phi_0 \rangle \propto \delta_{ij}$ for $1 \leq i, j \leq N-1$. The states a_i^* are uniquely determined from the state a_0^*. Ψ_Fr is a Slater state as well, consisting of $(n-1)$ single s-electron states a_i^* and a mixed s-d-state $(A a_0^* + B d^*)$.

In this paper I want to show that the theoretical proof of relation (5) is relatively straight forward if one uses a geometrical representation of the n-electron Slater state.

Let us assume that we have a Hamiltonian given in the basis of N single electron states c_ν^*. This basis defines

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an N-dimensional Hilbert space with the unit vectors $\mathbf{c}_\nu$. In this Hilbert space we consider n single electron states $e_1^*, ...e_n^*$ with $e_i^* = \sum_{\nu=1}^{N} \gamma_{i\nu} c_\nu^*$. We compose with these states an n-electron Slater state either by means of a Slater determinant or as a product of the n creation operators $\Psi_n = e_n^*...e_1^*\Phi_0$. In Hilbert space the n vectors $\mathbf{e}_i$ represent a basis for an n-dimensional subspace. We postulate: *The n-dimensional subspace is equivalent to the n-electron Slater state.* The weight or amplitude is equal to the volume of the n-dimensional parallelepiped which is defined by the vectors $\mathbf{e}_1, ...\mathbf{e}_n$. This means that a 1-dimensional electron state is equivalent to a 1-dimensional subspace of the Hilbert space, *i.e.*, a straight line defined by the single vector $\mathbf{e}_1$. (The usual definition of a single electron state as vector of length 1 in Hilbert space cannot be generalized to an n-electron state).

As an example I consider the following two 2-electron Slater states Ψ_{12} and Ψ'_{12}. The compositions of the 2-electron states are

a) Ψ_{12} is built from the two single electron states c_1^* and c_2^*, *i.e.*, $\Psi_{12} = c_2^* c_1^* \Phi_0$.

b) $\Psi'_{12}$is built from the two single electron states $\frac{1}{\sqrt{2}}(c_1^* + c_2^*)$ and $\frac{1}{\sqrt{2}}(c_1^* - c_2^*)$, *i.e.*, $\Psi'_{12} = \frac{1}{\sqrt{2}}(c_1^* + c_2^*)\frac{1}{\sqrt{2}}(c_1^* - c_2^*)\Phi_0$.

The two states Ψ_{12} and Ψ'_{12} are identical as a simple multiplication shows. But Ψ_{12} and Ψ'_{12} represent different parallelepipeds (squares) in the $\mathbf{c}_1$-$\mathbf{c}_2$ plane. However, the two vectors $[\mathbf{c}_2, \mathbf{c}_1]$ define the same plane as the two vectors $\left[\frac{1}{\sqrt{2}}(\mathbf{c}_1 + \mathbf{c}_2), \frac{1}{\sqrt{2}}(\mathbf{c}_1 - \mathbf{c}_2)\right]$. Any rotation of the two states c_1^* and c_2^* in this plane leaves the 2-electron Slater state unchanged. Therefore we confirm the postulate that Ψ_{12} is equivalent to the 2-dimensional subspace of the Hilbert space which is spanned by $\mathbf{c}_1, \mathbf{c}_2$ and the 2-dimensional volume of the parallelepiped $(\mathbf{c}_1, \mathbf{c}_2)$ gives the weight (amplitude) of this state.

This representation of the n-electron wave function emphasizes the fact that $e_n^*...e_1^*\Phi_0$ is just one representation of the state Ψ_n. Any other sub-basis of this subspace represents the same state. With this interpretation of an n-electron Slater state one can easily construct the new ground state Ψ_{Fr} of Friedel Hamiltonian. The general idea is the following: The traditional n-electron ground state Ψ_0 in equation (4) spans an n-dimensional subspace S_1 with the sub-basis ($\mathbf{b}_1$, $\mathbf{b}_2, ...,$ $\mathbf{b}_n$). By means of a rotation we construct a new sub-basis of S_1 which consists of $(n-1)$ s-states $\mathbf{a}_1, ..., \mathbf{a}_{n-1}$ and a mixed s-d-state $(A\mathbf{a}_0 + B\mathbf{d})$. This yields the state Ψ_{Fr} which is identical with Ψ_0. This procedure is now described in some detail.

The $(N+1)$ solutions b_i^* (Eq. (2)) of the Friedel Hamiltonian span a $(N+1)$ dimensional Hilbert space. The n-electron Slater state $\Psi_0 = \prod_{i=1}^{n} b_i^* \Phi_0$ is equivalent to the n dimensional subspace S_1.

In the new basis b_i^* the state d^* is given by

$$d^* = \sum_{i=1}^{N+1} A_i b_i^*.$$

Part of the vector $\mathbf{d}$ lies in the subspace S_1. This part is denoted as $\mathbf{d}'_1$ and the rest as $\mathbf{d}'_2$. We normalize these two vectors $\mathbf{d}_1 = \mathbf{d}'_1/|d'_1|$ and $\mathbf{d}_2 = \mathbf{d}'_2/|d'_2|$. The vectors $\mathbf{d}$ and $\mathbf{d}_1$ form an angle γ with $\cos\gamma = \sqrt{\sum_{i=1}^{n} A_i^2}$. Furthermore we have

$$\mathbf{d} = \mathbf{d}_1 \cos\gamma + \mathbf{d}_2 \sin\gamma.$$

Any vector in the subspace S_1 which is orthogonal to $\mathbf{d}_1$ is also orthogonal to $\mathbf{d}$, *i.e.*, it is composed of only the s-band states c_ν^*.

Now we can define the vector

$$\mathbf{a}_0 = -\mathbf{d}_1 \sin\gamma + \mathbf{d}_2 \cos\gamma.$$

This vector $\mathbf{a}_0$ is orthogonal to $\mathbf{d}$ and consists therefore only of s-states vectors $\mathbf{c}_\nu$. For $\mathbf{d}_1$ one obtains

$$\mathbf{d}_1 = -\sin\gamma \mathbf{a}_0 + \cos\gamma \mathbf{d}. \tag{7}$$

Unfortunately it is not possible to present the $(N+1)$ dimensional Hilbert space and its n-dimensional subspace graphically. However, to give some graphical assistance, the original basis vectors $(\mathbf{c}_1, ..., \mathbf{c}_N, \mathbf{d})$ as well as the basis vectors $(\mathbf{b}, ..., \mathbf{b}_{N+1})$ are shown in Figure 1 as linear arrays. They span the same Hilbert space and this is indicated by the shaded area between them.

All vectors in the subspace S_1 which are perpendicular to $\mathbf{d}_1$ are also perpendicular to $\mathbf{d}$. I choose now $\mathbf{d}_1$

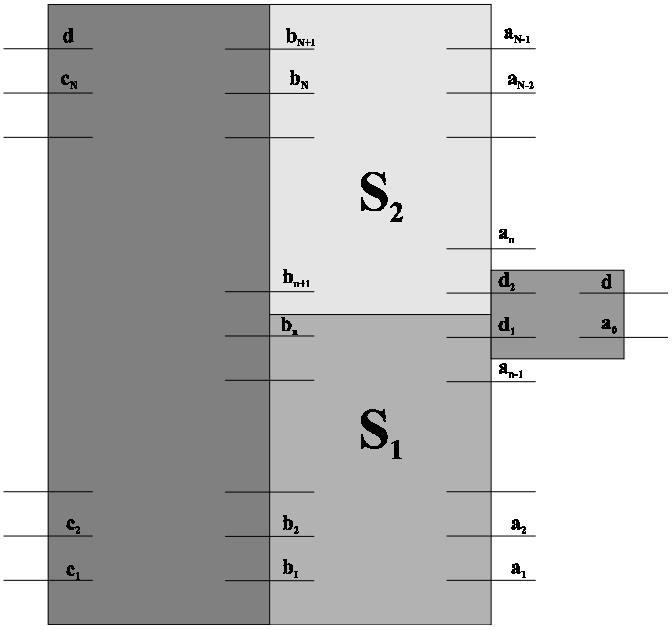

Fig. 1. The basis vectors $\mathbf{c}_1, ..., \mathbf{c}_N, \mathbf{d}$ span the $(N+1)$ dimensional Hilbert space. The same Hilbert space is spanned by the eigenvectors of the Friedel Hamiltonian $\mathbf{b}_1, ..., \mathbf{b}_{N+1}$. The n-dimensional subspace $\mathrm{S}_1 = \mathrm{S}(\mathbf{b}_1, ..., \mathbf{b}_n)$ is equivalent to $\mathrm{S}(\mathbf{a}_1, ..., \mathbf{a}_{n-1}, \mathbf{d}_1)$ while the orthogonal $(N+1-n)$ dimensional subspace $\mathrm{S}_2 = \mathrm{S}(\mathbf{b}_{n+1}, ..., \mathbf{b}_{N+1})$ is equivalent to $\mathrm{S}(\mathbf{d}_2, \mathbf{a}_n, ..., \mathbf{a}_{N-1})$. Furthermore the 2-dimensional subspace $\mathrm{S}(\mathbf{d}_1, \mathbf{d}_2)$ is equivalent to $\mathrm{S}(\mathbf{d}, \mathbf{a}_0)$. The shaded area between two columns of basis vectors indicates identical subspaces. As a consequence the corresponding multi-dimensional electron states are identical.

as one of the basis vectors in the S_1 subspace. The other $(n-1)$ basis states of S_1 are denoted as a_i^* $(0 < i \leq n-1)$. They are orthogonal to d_1^* and to each other (and can be constructed from the states b_j^*). Together with d_1 they define the n-dimensional subspace S_1. These states a_i^* are automatically orthogonal to d^* , *i.e.*, they are only composed of s-band states c_ν^*. A particular useful choice of the states a_i^* in the subspace S_1 is the one in which the s-band Hamiltonian $H_0 = \sum_{\nu=1}^{N} \epsilon_\nu c_\nu^* c_\nu$ has only diagonal matrix elements. This can be always achieved by a rotation in the $(n-1)$ dimensional subspace, *i.e.*, that part of S_1 that is orthogonal to $\mathbf{d}_1$.

In Figure 1 the third array of the new basis vectors $(\mathbf{a}_1, ..., \mathbf{a}_{n-1}, \mathbf{d}_1)$ is shown. Since they span the same subspace as $(\mathbf{b}_1,...,\mathbf{b}_n)$ the two sets of basis vectors is also connected by a shaded area. The other vectors will be discussed below.

In the second part of the proof it must be shown that one can complement the states a_i^* to a total of $(N-1)$ states which form (together with a_0^*) a full basis for the s-band and that their $(N-1)$ sub-matrix of the s-band Hamiltonian $H_0 = \sum_{\nu=1}^{N} \epsilon_\nu n_\nu$ is diagonal. For that purpose we consider the $(N-n+1)$ subspace S_2 which is spanned by the vectors $\mathbf{b}_{n+1}, ..., \mathbf{b}_{N+1}$. One basis vector of S_2 has already been defined and discussed above, the vector $\mathbf{d}_2$. The remaining $(N-n)$ dimensional subspace is orthogonal to S_1 and to $\mathbf{d}_2$ and is therefore also orthogonal to $\mathbf{d}$ (and $\mathbf{a}_0$)**.** One can construct $(N-n)$ ortho-normal basis vectors $\mathbf{a}_n, ..., \mathbf{a}_{N-1}$ (which consist only of s-states). These vectors are automatically orthogonal to **d.** As before in S_1 the sub-basis a_i^* $(n \leq i \leq N-1)$ can be rotated so that the $(N-n)$ sub-matrix of the s-band Hamiltonian H_0 is diagonal.

The basis vectors $\mathbf{a}_n, ...\mathbf{a}_{N-1}$ are orthogonal to $\mathbf{a}_1$, $...\mathbf{a}_{n-1}$. Furthermore we defined the $\mathbf{a}_i$ so that the s-band Hamiltonian H_0 is diagonal in each subspace. It is easy to show that matrix elements of H_0 between $\mathbf{a}_k$ in S_1 and $\mathbf{a}_l$ in S_2 vanish as well. (One expresses $\mathbf{a}_k$ and $\mathbf{a}_l$ in terms of $\mathbf{b}_j$).

Now we have $(N+1)$ basis vectors, consisting of $\mathbf{a}_1$, ..., $\mathbf{a}_{N-1}$ and $\mathbf{d}_1, \mathbf{d}_2$, where the vectors $\mathbf{a}_k$ are all orthogonal to $\mathbf{d}$ and the $(N-1)$ dimensional sub-matrix of H_0 is diagonal in this basis. The two basis vectors $\mathbf{d}_1, \mathbf{d}_2$ can be replaced by $\mathbf{a}_0$ and $\mathbf{d}$. In Figure 1 the basis vectors $\mathbf{b}_1, ..., \mathbf{b}_{N+1}$ are drawn as a linear array. The first n vectors span the subspace S_1 and the remaining $(N-n+1)$ span the subspace S_2. The same subspaces can be constructed by means of $\mathbf{a}_1, ..., \mathbf{a}_{n-1}, \mathbf{d}_1$ and $\mathbf{d}_2, \mathbf{a}_n, ..., \mathbf{a}_{N-1}$, *i.e.*:

$$\begin{aligned} \mathrm{S}(\mathbf{b}_1, ...\mathbf{b}_n) = \mathrm{S}(\mathbf{a}_1, ..., \mathbf{a}_{n-1}, \mathbf{d}_1) = \mathrm{S}_1 \\ \mathrm{S}\left(\mathbf{b}_{n+1}, ..., \mathbf{b}_{N+1}\right) = \mathrm{S}\left(\mathbf{d}_2, \mathbf{a}_n, ...\mathbf{a}_{N-1}\right) = \mathrm{S}_2 \\ \mathrm{S}(\mathbf{a}_0, \mathbf{d}) = \mathrm{S}(\mathbf{d}_1, \mathbf{d}_2). \end{aligned} \tag{8}$$

With these conclusions we have proven that the state Ψ_{Fr} in equation (5) is the n-electron ground state of the Friedel Hamiltonian, that the states $(a_1^*, ..., a_{N-1}^*)$ form (together with a_0^*) a new basis, that their sub-matrix of the s-band Hamiltonian is diagonal.

It is now easy to determine the exact form of the state a_0^* from the above conditions. One obtains

$$\begin{aligned} a_0^* = \frac{1}{\sin\gamma\cos\gamma} \sum_{\nu=1}^{N} \mathrm{c}_\nu^* \\ \times \left[\sum_{i=1}^{n} \beta_i \beta_{i\nu} \sin^2\gamma - \sum_{i=n+1}^{N+1} \beta_i \beta_{i\nu} \cos^2\gamma \right] \end{aligned} \tag{9}$$

where the coefficients β_i, $\beta_{i\nu}$ are given in equation (2). I compared these theoretical coefficients of the state a_0^* with the result of the numerical variation. They agree perfectly. However, the present result goes beyond the numerical result because it demonstrates that one can also express excited states in the form of equation (5).

References

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