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Coupling of conduction electrons to two-level systems formed by hydrogen: a scattering approach

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Abstract

An effective Hamiltonian for a two-level system (TLS) which could model the interaction between a tunneling proton and the conduction electrons of a metal is investigated in a comparative way. In the conventional first-order Born approximation with plane waves, and for small-distance displacement of the tunneling particle, a simple correlation between the atomic motion and angular momentum change of the scattering electron is deduced. For such a displacement, and within a distorted wave Born approximation for initial and final states, the change in the scattering amplitude is expressed via bounded trigonometric functions of the corresponding difference of scattering phase shifts. The numerical value of this amplitude change is analyzed in the framework of a self-consistent screening description for an impurity embedding in a paramagnetic electron gas. The coupling thus obtained of the tunneling proton to a homogeneous electron gas is too weak to be in the range required for realization of the two-channel Kondo effect.

1. Introduction

In the last few decades hydrogen in metals has deserved very extensive experimental studies and vast theoretical considerations. In crystalline solids the hydrogen (H) sits in a well-defined interatomic position like, for example, in Pd or Pt. That is not the case in amorphous systems and at dislocations and other nonperiodic distortions. If the H has some more room between the host atoms its position may not be well defined and it moves between two positions. Such systems are known as two-level systems (TLS) and they have been very extensively studied [1]. The coupling to the conduction electrons can result in an extra contribution to the electrical resistivity [2]. If the atom has two metastable positions the electron scattering amplitude in different angular momentum channels depends on the atomic position. The difference between these amplitudes is described in the literature by a coupling V^z . That coupling contributes to the resistivity in a conventional way.

There are, however, other couplings where electrons induce transitions between the two levels. Thus an assisted transition can be realized by the tunneling of the atom between the two positions [3–5]. The importance of that coupling,

denoted by V^x and V^y , is highly debated [6, 7]. These models consider different atoms with sizable differences in their masses. The original suggestion is limited to small tunneling rate, while more intensive tunneling induces an essential split between the energies of the atomic eigenstates which reduces their roles. The model has attracted considerable interest as it was suggested that at low temperature it exhibits the non-Fermi liquid behavior known as the two-channel Kondo (2CK) effect, which has its own theoretical interest [8, 9].

Experimental support comes much more from the studies of point contacts than from direct measurement of the electrical resistivity [8]. The Cornell group made a detailed suggestion how the observed zero-bias anomalies could be due to that 2CK effect, which has also been highly debated [6]. Since that time the original model was modified [7] by taking into account the actual electronic structure at the TLS. The possibility was also considered [10] where the atom moves between the two positions via the next higher energy level of the atomic motion. These suggestions were aimed to increase the electron-assisted amplitudes (V^x , V^y) to make the 2CK more feasible. The enhancement of these couplings by the renormalization due to the conduction electrons is driven by V^z . The estimated

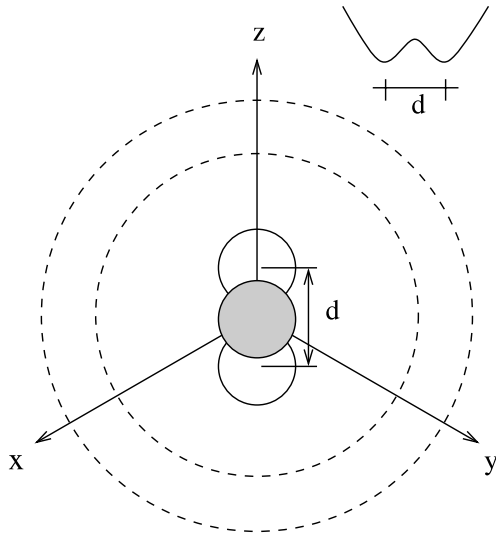


Figure 1. Illustration of the two-level system. The shadowed circle represents the screened proton in the central position and the two others, separated by d , the TLS. The dashed lines correspond to the spherical wave centered around the origin. The inset shows the potential of the TLS.

couplings were on the borderline and therefore those should be studied in more detail. It is crucial whether those coupling strengths could reach certain regions which are very sensitive to the strength of V^z .

Motivated by this important role of a V^z input to dimensionless scaling equations, the present paper is devoted to a consistent determination of its magnitude within scattering theory. This is the main goal of our work, in which the tunneling-related other couplings (and thus their feedback effects in scalings) are not investigated. In order to achieve this goal, we consider a heavy atom (hydrogen) which has two stable positions (separated on the atomic scale) in a metallic matrix due to a double potential well. The positions are symmetric round a central point and they are at $z = \pm \frac{d}{2}$, respectively; see figure 1 for illustration. These positions are described by a pseudospin $\sigma^z = \pm 1$. As a possible application of our work, the problem of zero-bias anomaly found [11] in hydrogenated palladium contacts can be mentioned.

The general form of the Hamiltonian is $H = H_0 + H_1$, where the diagonal H_0 matrix stands for independent electrons in stationary eigenstates of a self-consistent external field $V(r)$ generated by the embedded (at $z = 0$) particle in the electron gas:

$$H_0 = \sum_{\gamma, \sigma} \varepsilon_\gamma a_{\gamma\sigma}^\dagger a_{\gamma\sigma}, \quad (1)$$

in which the ε_γ are energy eigenvalues of bound and scattering eigenstates. The $a_{\gamma\sigma}^\dagger$ and $a_{\gamma\sigma}$ create and annihilate, respectively, these eigenstates of equation (1) of spin σ . In order to construct H_1 in a physically consistent way in our modeling, we shall consider (see section 2.2) a perturbation $[\Delta V(\mathbf{r})]$ which is due to the shift in the atomic position. We stress that, within the framework of such modeling, it is customary in the TLS literature [5, 9, 10] to approximate the scattering eigenstates by plane waves (pw). Based on this

a priori assumption (neglecting $V(r)$ in H_0) for initial and final states, one can write $H_1^{(pw)}$ as

$$H_1^{(pw)} = \sigma^z \frac{1}{V} \sum_{\mathbf{q}} V_{pw}^z(\mathbf{q}) \sum_{\mathbf{p}} b_{\mathbf{p}+\mathbf{q}}^\dagger b_{\mathbf{p}}, \quad (2)$$

with the corresponding operators for the creation and annihilation of plane-wave states. Here we have $\mathbf{q} = \mathbf{k}_2 - \mathbf{k}_1$, and thus $V_{pw}^z(\mathbf{q})$ is given by

$$V_{pw}^z(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \Delta V(\mathbf{r}). \quad (3)$$

Since the perturbation, $\Delta V(\mathbf{r})$, is real we have $[V_{pw}^z(\mathbf{q})]^* = V_{pw}^z(-\mathbf{q})$, i.e. the $H_1^{(pw)}$ is Hermitian. The scattering-amplitude change is simply $\Delta F_{pw}^z(\mathbf{q}) = [m/(2\pi\hbar^2)]V_{pw}^z(\mathbf{q})$.

Of course, if the self-consistent external field, $V(r)$, is not weak one must calculate the corresponding scattering amplitude change $[\Delta F^z(\mathbf{k}_2, \mathbf{k}_1)]$ by using properly defined [12, 13] initial and final states instead of plane waves. The nontrivial role of incorporating the static central potential in the electronic wavefunctions has already [10] been pointed out by arguing that the effect of $V(r)$ can be quite important. Namely, the possible role of a renormalized density of states, $\rho_0 \rightarrow \rho_0 \cos^2(\delta_0)$, in the final coupling is mentioned. In a similar way, a possible double effect [7], i.e. the matrix element of a potential gradient together with the square root of a modified density of states, has also been discussed using an *unscreened* Coulomb potential to calculate a matrix element (cf [13]).

In the present paper we implement the following construction [4] for the interaction energy:

$$H_1 = \sigma^z \frac{1}{V} \sum_{\mathbf{k}_1, \mathbf{k}_2} V_{\mathbf{k}_2, \mathbf{k}_1}^z a_{\mathbf{k}_2, \sigma}^\dagger a_{\mathbf{k}_1, \sigma}, \quad (4)$$

where the suitable coupling $V_{\mathbf{k}_2, \mathbf{k}_1}^z = \sum_{\alpha\beta} f_\beta^*(\hat{k}_2) V_{\alpha\beta}^z(k_1, k_2) f_\alpha(\hat{k}_1)$ is Hermitian. In this representation [4, 5, 9] the $f_{lm}(\hat{k}) = i^l \sqrt{4\pi} Y_{lm}(\hat{k})$ functions are spherical harmonics; α and β run over a properly chosen set of angular momentum indices (l, m). We note here for completeness that the magnetic spin σ will play no direct role in the coupling to the TLS. It plays the role of an additional channel index [9] required in a two-channel Kondo model.

We determine, in a consistent manner, the change $[\Delta F_{\alpha\beta}^z(\mathbf{k}_2, \mathbf{k}_1)]$ in the electron scattering amplitude in different angular momentum channels when the *screened* heavy particle is moved out from the central point to one of the two positions, but the set of the electron wavefunctions is still centered at the origin. These functions are calculated in a self-consistent Hartree-like manner using density-functional theory for a proton embedding in an electron gas of given density n_0 . Thus the change in the scattering amplitude, due to a potential displacement $\Delta V(\mathbf{r})$, is expressed in the distorted wave Born approximation [12, 13] via matrix elements taken between precalculated scattering eigenstates of H_0 . Then we connect $\Delta F_{\alpha\beta}^z(\mathbf{k}_2, \mathbf{k}_1)$ with $V_{\alpha\beta}^z(k_1, k_2)$, considering the required Hermitian character. In such a manner, we obtain a *bounded* function for the dimensionless coupling in terms of

scattering phase shifts determined self-consistently. This is our main result in this work.

The rest of this paper is organized as follows. Section 2 contains our theory in the form of subsections organized around the key elements of a consistent attempt. In order to provide a clear phenomenology to the problem of a TLS modeled by a mobile atom in a metallic system, the plane-wave-based Born approximation, i.e. the basis of earlier attempts [5, 9, 10] in V^z estimations, is also discussed in a comparative way. Section 3 is devoted to a short summary. The appendix summarizes the elements of the tangent method applied previously to the effect of strong scattering.

2. Theory and results

The present comparative study on a suitable [4] coupling is carried out in several steps, as we mentioned above. In order to get an *a posteriori* statement on the effect of the external field, we start with the analysis of $V(r)$ and its scattering characteristics.

2.1. Calculations of the screened potential around the proton and the phase shifts

The charge (Z) is sitting in the central position where its screened field $V(r)$ and a complete set of one-electron wavefunctions of occupied states are determined in a self-consistent way by applying the Kohn–Sham method [15] of density-functional theory (DFT) with the local-density approximation (LDA) for the induced exchange–correlation potential. Briefly, the single-particle potential energy $V(r)$ has a simple form in this approximation:

$$V(r) = -\frac{Ze^2}{r} + \int d^3\mathbf{r}' \frac{\Delta n(r')}{|\mathbf{r} - \mathbf{r}'|} + \Delta v_{xc}[n(r)], \quad (5)$$

in which $\Delta n(r)$ is the screening density. The many-body term $\Delta v_{xc}[n]$ is expressed via an input exchange–correlation chemical potential (μ_{xc}) as $\Delta v_{xc}[n] = \mu_{xc}(n_0 + \Delta n) - \mu_{xc}(n_0)$ in LDA. In our treatment we have a vanishing effective potential energy at infinity.

For a given density (n_0) of the screening environment, and depending on the magnitude of the attractive embedded charge, the total density consists of bound and scattering eigenstates. The $n(r) = n_0 + \Delta n(r)$ total density, the basic variable of DFT, is constructed by summing over doubly occupied bound and scattering-like states:

$$\psi_{\mathbf{k}}^{\pm}(\mathbf{r}) = \sqrt{4\pi} \sum_{lm} A_l(k) R_l(k, r) Y_{lm}^*(\hat{r}) f_{lm}(\hat{k}), \quad (6)$$

in which $R_l(k, r)$ are solutions of the radial Kohn–Sham equations with $V(r)$ at $(\hbar k)^2/2m$ scattering energy and $A_l(k) = e^{\pm i\delta_l(k)}$, where $\delta_l(k)$ is the phase shift; $f_{lm}(\hat{k})$ was introduced in equation (4). The continuum states are normalized on the k scale. Thus the scattering (sc) part of the induced density comes from an integral over the Fermi–Dirac distribution function:

$$\Delta n_{sc}(r) = \frac{1}{\pi^2} \sum_{l=0}^{\infty} (2l+1) \int_0^{k_F} dk k^2 [R_l^2(k, r) - j_l^2(kr)]. \quad (7)$$

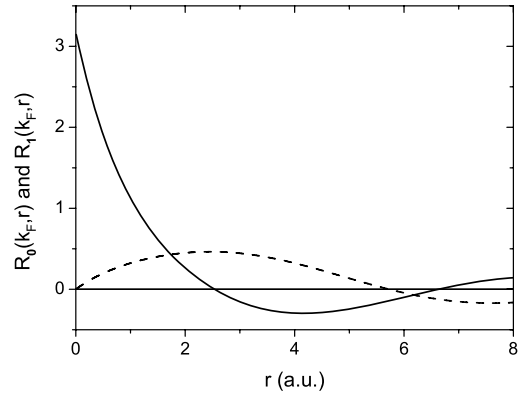


Figure 2. Self-consistently determined radial wavefunctions, $R_0(k_F, r)$ and $R_1(k_F, r)$, as a function of the radial distance r in atomic units (au). Solid and dashed curves refer, respectively, to the $l = 0$ and 1 components. The Wigner–Seitz parameter of the host system is $r_s = 2.5$ (au).

The total screening condition, $4\pi \int_0^{\infty} dr r^2 \Delta n(r) = Z$, implies the Friedel sum rule of scattering phase shifts in a one-electron mean-field treatment:

$$Z = \frac{2}{\pi} \sum_{l=0}^{\infty} (2l+1) \delta_l(k_F) - \frac{2}{\pi} \sum_{l=0}^{\infty} (2l+1) \delta_l(0) + N_b. \quad (8)$$

Here N_b denotes the number of occupied bound states, and in a ground-state calculation the last two terms cancel each other according to Levinson’s theorem. At metallic densities, the first few phase shifts already provide a very accurate [16, 17] approximation. For protons ($Z = 1$), at the $r_s = 2.5$ value of the density parameter one has $\delta_0(k_F) = 1.2213$ and $\delta_1(k_F) = 0.0894$. This r_s value can characterize [18] the electron fluid of a Pd metal.

Illustrative results are shown in figure 2 for the leading, $l = 0$ and 1, radial wavefunctions calculated at the $r_s = 2.5$ value of the Wigner–Seitz parameter. The $l = 0$ component shows a remarkable Coulomb-like enhancement, $\sqrt{2\pi}/k_F$, at the origin $r = 0$, over the plane-wave-based unity. There are marked deviations from the plane-wave components $j_0(k_F r)$ and $j_1(k_F r)$, as figure 3 shows via the corresponding products of components. Based on these important characteristics, we can conclude that the attractive proton is a strong *local* perturbation at metallic densities. This *a posteriori* conclusion signals that the effect of $V(r)$ in H_0 is, in a treatment of quantitative quality, not negligible.

Now, we connect the above local environment picture with the proposal of Hopfield [19] for short-range properties when there is a *change* in the potential due to moving an atom by a small distance. It was shown that *when* an angular momentum decomposition of electron wavefunctions is used, the matrix elements contain chiefly scatterings which change the angular momentum of the electron. Precisely, it is this character which is central in the context of the scattering of electrons from two-level systems. The parity change of the angular momentum state, without altering the spin indices, of conduction electrons gives them an internal degree of freedom coupled to that of the impurity [4, 20]. This internal degree is the background

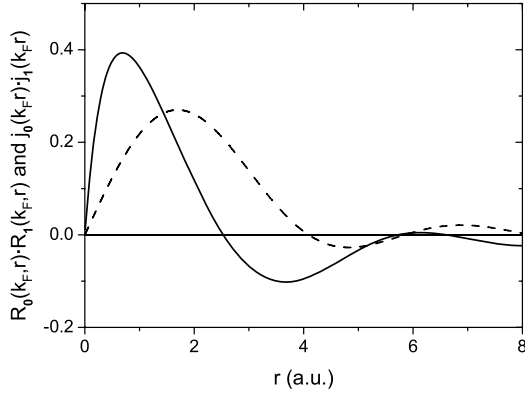


Figure 3. Products of the leading partial waves as a function of r . The solid and dashed curves correspond, respectively, to the self-consistent $R_0(k_F, r)R_1(k_F, r)$ and the perturbative $j_0(k_F r)j_1(k_F r)$. The Wigner–Seitz parameter of the host system is $r_s = 2.5$ (au).

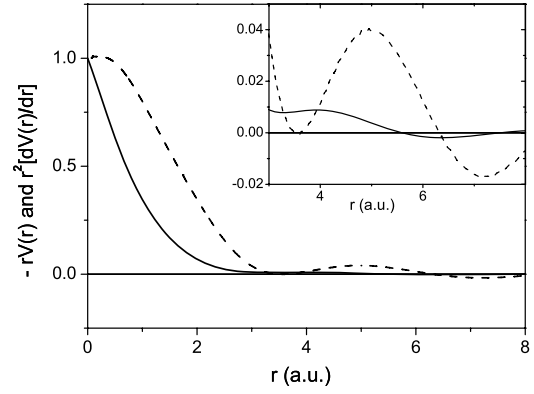


Figure 4. Characteristics of the self-consistent potential obtained at $r_s = 2.5$ within DFT for the screening of a proton. The $-rV(r)$ and $r^2[dV(r)/dr]$ are plotted as a function of r by solid and dashed curves, respectively. The inset is devoted to finer details for $r > 3$. Atomic units are used.

to establish an analogy with the usual (spin-related, magnetic) Kondo effect.

2.2. The change of the potential for $d \neq 0$

As we explained in section 1, the screened charge is moved to one of the positions $\sigma^z = \pm 1$ carrying the potential, which is taken rigid, as the screening action is very fast [21, 22] compared to the infrared processes essential in some other problems. The electron eigenfunctions are carried with the tunneling atom, but they are decomposed in terms of those that have already been determined for the central position with $V(r)$. The perturbing potential is defined as

$$\sigma^z \Delta V(\mathbf{r}) = V(\mathbf{r}) - V\left(\mathbf{r} - \sigma^z \frac{d}{2} \hat{z}\right) \quad (9)$$

and thus the important term in further discussion becomes

$$\Delta V(\mathbf{r}) \Rightarrow \frac{d}{2} \frac{\partial V(\mathbf{r})}{\partial r_z} = \frac{d}{2} \cos \theta \frac{dV(r)}{dr}, \quad (10)$$

in the physically reasonable small- d limit. We illustrate the self-consistent potential and its gradient in figure 4. The products of $-rV(r)$ and $r^2[dV(r)/dr]$ are plotted by solid and dashed curves, respectively. The inset is devoted to the finer details of these functions. The Coulombic character of $r^2[dV(r)/dr]$ at short distance is due to a compensating effect between the Hartree term and the exchange–correlation term treated here within the LDA.

As a next step in our comparative study, perturbation theories are applied in terms of $\Delta V(\mathbf{r})$. The matrix elements are calculated between the states with wavefunctions $\psi_{\mathbf{k}}^{\pm}(\mathbf{r})$ determined in section 2.1, but with the plane wavefunctions also presented to establish a proper phenomenology. In other words, we use the distorted wave Born and the conventional (plane-wave-based) Born approximations [12, 13], respectively.

2.3. Matrix elements of the shifted potential between the original wavefunctions

In order to get a convenient, dimensionless [5] coupling to characterize the effect of the perturbation we shall use energy normalization [23] for scattering states:

$$\psi_E(\mathbf{r}) = \frac{1}{\sqrt{4\pi}} \sqrt{\frac{2mk}{\pi \hbar^2}} \psi_{\mathbf{k}}(\mathbf{r}). \quad (11)$$

The original matrix element at k_F is multiplied in such a way by the density of states $\rho_0(E_F) = (k_F m)/(2\pi^2 \hbar^2) = 0.75n_0/E_F$ per unit volume for a given spin evaluated at the Fermi energy. Notice, once more, that the $\Delta F^z(\mathbf{k}_1, \mathbf{k}_2)$ change in the scattering amplitude, i.e. the matrix element of the perturbing $\Delta V(\mathbf{r})$ between $\psi_{\mathbf{k}}^{\pm}(\mathbf{r})$ initial and final states [12] of equation (6), should involve a $m/(2\pi \hbar^2)$ prefactor. With our $\Delta V(\mathbf{r})$ the angle integration over $\Omega_{\hat{r}}$ gives, by applying the standard recurrence relation for $\cos \theta Y_{lm}(\theta, \phi)$, the simple result

$$I(l, m) = \int d\Omega_{\hat{r}} \cos \theta Y_{lm}(\hat{r}) Y_{l'm'}^*(\hat{r}) = \left[\frac{(l+1)^2 - m^2}{4(l+1)^2 - 1} \right]^{1/2}. \quad (12)$$

Only the $l' = l + 1$ and $m' = m$ values are allowed, due to the dipolar character.

Born approximation. Motivated by the previous [5, 9, 10] TLS literature, and to get a further *a posteriori* statement, first we study the case of a weak $V_{ps}(r)$ pseudo-potential to equation (10). Thus, we perform the radial integration in the matrix element determination by applying plane-wave components for the free (cf equation (6)) radial wavefunctions as

$$I_k(l) = \frac{2m}{\hbar^2} \int_0^\infty dr r^2 \frac{dV_{ps}(r)}{dr} j_l(kr) j_{l+1}(kr), \quad (13)$$

in the knowledge of the simple selection rule obtained above in angle integration. In this perturbative case the integration by

parts and use of the following expression based on recurrence relations for Bessel functions:

$$\frac{d}{dr} [r^2 j_l(k_1 r) j_{l+1}(k_2 r)] \equiv r^2 [k_2 j_l^2(k_1 r) - k_1 j_{l+1}^2(k_2 r)], \quad (14)$$

results in a remaining integral with $V_{ps}(r)$. Now, we apply the standard definition [12] of the first-order Born (B) phase shift:

$$\delta_l^B(k) = -\frac{2mk}{\hbar^2} \int_0^\infty dr r^2 V_{ps}(r) j_l^2(kr), \quad (15)$$

to obtain the following informative (cf equation (18), below) expression:

$$I_k^B(l) = [\delta_l^B(k) - \delta_{l+1}^B(k)]. \quad (16)$$

We stress that this equation is valid, physically, only for small values of the phase shifts, i.e. when the distortion of the electron wavefunction by the central potential field is negligible. However, and this is the real message based on the detailed algebra given above, the proposed correlation [4] between the motion of the TLS atom and an angular momentum *change* is transparent ($\alpha \Rightarrow l$ and $\beta \Rightarrow (l+1)$) to equation (4) already at the first-order Born level.

Beyond the first-order Born approximation. In a quite recent theoretical work [7], which also rests on the matrix element calculation with a potential gradient between normalized s and p *bound* states, the bare $[V_C(r) = -Z/r]$ Coulomb potential was applied to characterize the TLS in a metallic matrix. Here, using the $\eta = Ze^2 m / (k\hbar^2)$ Sommerfeld parameter, we add the corresponding *exact* phase shift difference for the case of a Coulomb field:

$$\delta_l^C(k) - \delta_{l+1}^C(k) = \arctan \left[\frac{\eta}{(l+1)} \right]. \quad (17)$$

It is to be noted at this point that, despite the simplicity of this expression, the application of results based on a bare Coulomb field has a limited validity in the problem under discussion since the screening action of mobile electrons is important. On the other hand, by using the accurate $R_l(k, r)$ and $R_{l+1}(k, r)$ radial wavefunctions in the integration in equation (13) with the gradient of the true $V(r)$ behind these functions one still obtains [24, 25] a closed

$$I_k(l) = \sin[\delta_l(k) - \delta_{l+1}(k)] \equiv [\tan \delta_l(k) - \tan \delta_{l+1}(k)] \times \cos \delta_l(k) \cos \delta_{l+1}(k), \quad (18)$$

expression in terms of scattering phase shifts. This exact result, which now contains precisely the effect of the central potential field at the level of self-consistency, is a *bounded* function in contrast to equation (16). Of course, for small phase shifts equation (18) reduces to the perturbative (plane-wave-based) result given by equation (16).

We illustrate, in figure 5, the argument function $r^2 R_0(k_F, r) R_1(k_F, r) [dV(r)/dr]$ of equation (13) by using the self-consistent solutions at $r_s = 2.5$. Fortunately, we have already an *analytic* result in equation (18) for the integral. Notice that a formal application of the standing wave boundary condition (see the appendix) would result in the rhs of equation (18) *only* with the difference of tangents due to the standard $e^{i\delta_l(k)} \Rightarrow 1/\cos \delta_l(k)$ change in normalization.

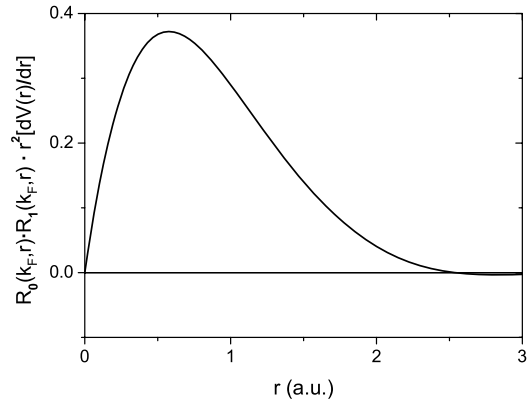


Figure 5. Illustration of the integrand of equation (16) obtained by using the self-consistent result for the potential gradient and the two leading radial wavefunctions. The Wigner–Seitz parameter of the host system is $r_s = 2.5$. Atomic units are used.

2.4. Dimensionless matrix element and scattering-amplitude change

After the derivation of $\Delta F_{\alpha\beta}^z(k_1, k_2)$ channel terms to the total amplitude change, denoted as $\Delta F^z(\mathbf{k}_1, \mathbf{k}_2)$, we turn our attention to the matrix element [4] needed (at the Fermi level) for a suitable coupling introduced in equation (4). To find the link, and follow our comparative method, first we give a *dimensionless* expression which characterizes the *partial* amplitude change:

$$\begin{aligned} \Delta f_{\alpha\beta}^z(k_F) &\equiv (k_F/\pi) \Delta F_{\alpha\beta}^z(k_F) \\ &= \frac{d}{\lambda_B} I(l, m) I_{k_F}(l) A_{l+1}(k_F) A_l(k_F), \end{aligned} \quad (19)$$

in which $\lambda_B = 2\pi\hbar/p_F$ for convenience, and α and β refer (see above) to the (l, m) and $(l+1, m)$ values, respectively. Next, following earlier works [4, 5, 9], we write a dimensionless form for the Hermitian H_1 in equation (4) as

$$v_{\alpha\beta}^z(k_F) \equiv \rho_0(E_F) V_{\alpha\beta}^z(k_F). \quad (20)$$

The obvious link is simply $v_{\alpha\beta}^{z(B)}(k_F) = \Delta f_{\alpha\beta}^{z(B)}(k_F)$ in the plane-wave-based Born (B) approximation, since with plane waves (pw) for initial and final states one has $V_{pw}^z(k_F) \sim \Delta F_{pw}^z(k_F)$ as we explained already for equation (3) in section 1.

This transparent connection between physical quantities at the Fermi surface suggests us to use, beyond the weak coupling limit above, the $v_{\alpha\beta}^z(k_F) = \text{Re} \Delta f_{\alpha\beta}^z(k_F)$ extension. With our choice for boundary conditions to select initial and final states, involved in matrix element calculation based on the distorted wave Born method, this seems to be the only logical step which preserves the important Hermitian character of H_1 and reproduces the weak coupling limit. This extension is in complete harmony with the standard textbook statement [26] on an energy *shift* of a particle interacting with a potential. We can write

$$\begin{aligned} \text{Re} \Delta f_{00,10}^z(k_F) &= \frac{1}{\sqrt{3}} \frac{d}{\lambda_B} \sin[\delta_0(k_F) - \delta_1(k_F)] \\ &\quad \times \cos[\delta_0(k_F) + \delta_1(k_F)], \end{aligned} \quad (21)$$

$$\begin{aligned} \text{Im } \Delta f_{00,10}^z(k_F) &= \frac{1}{\sqrt{3}} \frac{d}{\lambda_B} \sin[\delta_0(k_F) - \delta_1(k_F)] \\ &\times \sin[\delta_0(k_F) + \delta_1(k_F)] \end{aligned} \quad (22)$$

for the important real (Re) part and the imaginary (Im) part. This latter is at least second order in a weak-perturbation ($Z \rightarrow 0$) limit.

The expression for the real part is the main result of our comparative study. In contrast to the conventional Born approximation, we have a *bounded* function in terms of self-consistent phase shifts for the Hermitian coupling. In the unitary limit, $\delta_0(k_F) \sim \pi/2$, where the effect of the self-consistent central $V(r)$ field is strong (see figures 2 and 3), the influence of the potential shift $[\Delta V(\mathbf{r})]$ becomes very small, i.e. $v_{00,10}^z(k_F)$ is small. This observation is in accord with an earlier conclusion [27] on a renormalized limit, obtained via mapping to the partition function of an auxiliary logarithmic gas, with contact interaction.

We note, finally, that the expression in equation (19) is linear in d , since it is based on the leading-term expansion, indicated in equation (10), for the perturbation. In order to get a more detailed d dependence, we performed numerical volume integrations with $\Delta V(\mathbf{r})$ from equation (9) and the *dominating* $R_0(k_F, r)Y_{00}(\hat{r})R_1(k_F, r)Y_{10}(\hat{r})$ product. By introducing the notation

$$K^z(d) \equiv |\Delta f_{00,10}^z(k_F)|\lambda_B, \quad (23)$$

and performing the θ integration via a variable change, we have

$$\begin{aligned} K^z(d) &= \frac{2\sqrt{3}}{d^2} \int_0^\infty dr R_0(k_F, r)R_1(k_F, r) \\ &\times \int_{|r-d/2|}^{r+d/2} du u V(u)[r^2 + (d/2)^2 - u^2]. \end{aligned} \quad (24)$$

The numerical result for $K^z(d)$ is presented in figure 6 by a solid curve. The dashed curve refers to the asymptotic expansion, which is linear in d . The illustrative figure shows that an asymptotic expansion provides a quite acceptable representation up to about $d \simeq 0.5$. Even at the physically reasonable $d = 1$ maximal value for a shift, the deviation from the numerical results is only about 25%.

The magnitude of $|\Delta f_{00,10}^z(k_F)|$ can be evaluated by using our phase shifts at density parameter $r_s = 2.5$, i.e. $k_F \simeq 0.77$, and assuming $d = 1$ for the size of the TLS and then

$$|\Delta f_{00,10}^z(k_F)| = \frac{k_F}{2\pi} K^z(d = 1) \simeq 0.05. \quad (25)$$

This value is in accordance with the typical values *estimated* earlier [2, 28] for different metallic glassy systems in the intermediate coupling regions using data of ultrasound measurements. Thus the coupling based on the present nonperturbative treatment is too weak to be in the range required (see the appendix) for the realization of the two-channel Kondo effect.

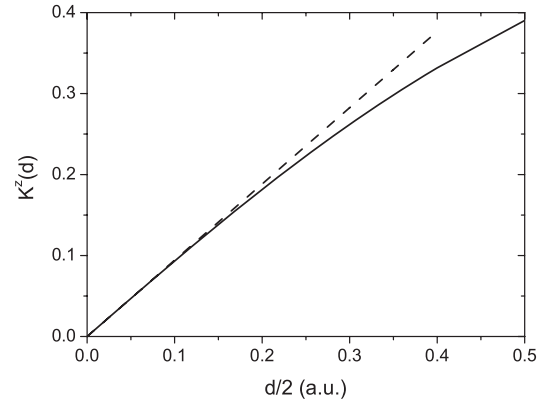


Figure 6. Numerical result (solid curve) for $K^z(d)$, defined in equation (27), as a function of $(d/2)$. The dashed curve refers to the asymptotic Taylor expansion which gives a linear dependence on d . The Wigner–Seitz parameter of the host system is $r_s = 2.5$. Atomic units are used.

3. Summary

A dimensionless coupling constant that characterizes the effect of a potential-gradient perturbation on scattering eigenstates of a self-consistently treated embedded impurity is deduced for small values of the impurity displacement d in metallic electron gases. The result is expressed via bounded trigonometric functions of scattering phase shift differences at the Fermi energy. The bounded character for a residual coupling shows that conventional, plane-wave-based, earlier estimations for this coupling are of restricted validity. Our main result, given by equations (20) and (21), can give a proper phenomenology in the theory of the TLS problem.

Beyond the applied distorted wave Born approximation, and with an axially symmetric scattering potential, the exact description would lead to *coupled* radial equations [29] in a partial wave expansion of the scattered wave at a given k . The d dependence of the coupling could be an exciting theoretical problem in such a treatment. Finally, a way to consider electronic inhomogeneities in a real host could be an *additional* local-density approximation. The strong local distortion by an embedded proton may justify such an approximation.

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Appendix. The tangent method

In the case of a contact $\bar{V}_0\delta(\mathbf{r})$ auxiliary interaction, which gives a constant potential in momentum space, one has the $\tan \bar{\delta}_0 = -\pi\rho_0\bar{V}_0$ simple form for the s-wave phase shift.

The standing (st) wave solution of the underlying [30] tangent method is given by

$$\phi_{\text{st}}(k_F, r) = \frac{1}{\cos \bar{\delta}_0} \frac{\sin(k_F r + \bar{\delta}_0)}{k_F r}, \quad (26)$$

while the solution with outgoing boundary condition has the form of

$$\psi^+(k_F, r) = e^{i\bar{\delta}_0} \frac{\sin(k_F r + \bar{\delta}_0)}{k_F r}. \quad (27)$$

The role of different normalizations, on which our previous statement at equation (18) is based, is apparent in these solutions.

The *standard* logic to determine a value of \bar{V}_0 is based on the phase shift $[\delta_0(k)]$ of the real potential $[V_0(r)]$, but the s -channel contact interaction has an important limitation when we apply it to the screening problem of a charge Z . It was pointed out [31] that this model cannot supply enough charge to shield the Coulomb field of the physically simplest impurity $Z = 1$. A *formal* requirement of $\delta_0(k_F) = \bar{\delta}_0$ would result in $\bar{V}_0 \rightarrow \infty$, when the self-consistent $[\delta_0(k_F)]$ leading phase shift (for $Z = 1$) goes to $\pi/2$.

The auxiliary contact potential was applied earlier [32] in an *opposite* way, i.e. via a direct approximation ($\bar{V}_0 \sim d$), for it to characterize the (constant) momentum-space potential of an atomic displacement in a free electron gas. In this case $\tan \bar{\delta}_0$ could measure a renormalized effect of a prefixed \bar{V}_0 , beyond the conventional (plane-wave-based) Born approximation where $\bar{\delta}_0^{(B)} = -\pi \rho_0 \bar{V}_0$. As we mentioned in section 1, a renormalized density of states $[\rho_0 \rightarrow \rho_0 \cos^2(\bar{\delta}_0)]$ could modify [10] the $\tan \bar{\delta}_0$ value. Its incorporation could reduce the final coupling, in agreement with our main result given by equations (20) and (21).

The direct approximation was implemented [7] earlier as $\tan \bar{\delta}_0 \equiv \pi v^z$ with a dimensionless matrix element $[(v^z/\sqrt{\rho_0}) \sim d]$ of the Coulomb potential gradient of an embedded proton taken between the corresponding hydrogenic (1s and 2p) bound states. The additional analysis, based on nonperturbative scaling equations [33], shows that there is a critical value ($v^z = 1/\pi$) for the input coupling. Only for a higher v^z could [14] the physics of the tunneling system be dominated [7] by the two-channel Kondo fixed point.

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