PHYSICAL REVIEW B **78**, 195124 (2008)

Friedel oscillations near Kondo impurities: A comparison of numerical calculation methods

Gerd Bergmann[*]

Department of Physics, University of Southern California, Los Angeles, California 90089-0484, USA

(Received 17 June 2008; revised manuscript received 1 September 2008; published 25 November 2008)

Recently, Affleck *et al.* derived the existence of Friedel oscillations in the presence of a Kondo impurity. They supported their analytic derivation by numerical calculations using Wilson's numerical renormalization group (NRG). In this paper the size of the Friedel oscillations is calculated with the Friedel artificially inserted resonance (FAIR) method which has been recently developed. The results of NRG and FAIR are compared. The development of Friedel oscillations with a phase shift of $\pi/2$ outside of the Kondo radius is confirmed.

DOI: 10.1103/PhysRevB.78.195124 PACS number(s): 75.20.Hr, 71.23.An, 71.27.+a

The properties of magnetic impurities in a metal is a fascinating problem which was first studied by Friedel[1] and Anderson.[2] The disappearance of the magnetic moment at low temperatures, the Kondo effect, is one of the most intensively studied problems in solid-state physics.[3–18] In the last decade the Kondo effect has experienced a renaissance. There is a growing interest in this field,[19] extending from magnetic atoms on the surface of corrals[20] to carbon nanotubes,[21] quantum dots,[22–28] and nanostructures.[29] There are still many open questions, particularly the real-space form of the wave function and the resulting charge density and polarization.

Recently Affleck, Borda, and Saleur[30] (ABS) investigated the formation of Friedel oscillations in the vicinity of a Kondo impurity. Their result has the form

$$\rho_{\mathrm{Fr}}(r)-\rho_0=\frac{C_D}{r^D}\left[F\left(\frac{r}{r_K}\right)\cos\left(2k_F r-D\frac{\pi}{2}\right)-\cos\left(2k_F r-D\frac{\pi}{2}\right)\right], \tag{1}$$

where D is the dimension of the system, the coefficients C_D have the values $C_1=1/(2\pi)$, $C_2=1/(2\pi^2)$, and $C_3=1/(4\pi^2)$, and $r_K=\hbar v_F/k_B T_K$ is the Kondo length. The function $F(r/r_K)$ is a universal function which approaches the values +1 for $r/r_K \ll 1$ and −1 for $r/r_K \gg 1$. (I skipped the phase shift δ_P due to potential scattering).

Besides the analytic derivation of Eq. (1) ABS performed also numerical calculations using Wilson's numerical renormalization group (NRG) approach.[11] In the NRG technique one uses Wilson states with a logarithmic discretization of the conduction band [which extends from $(-1,+1)$ (in units of the Fermi energy) and has a constant density of states].

ABS pointed out that Wilson energy states are not well suited for the calculation of such fine effects as Friedel oscillations. The reason is that the Wilson states average over a large number of original **k** states. Therefore they used a modified method which was introduced earlier by Borda (for details see Ref. 26). With this approach they obtained a numerical confirmation of the universal function $F(r/\xi_K)$.

The author has introduced, during the past few years, a new numerical approach to the Kondo and the Friedel-Anderson impurity, the Friedel artificially inserted resonance (FAIR) method. It is based on the fact that the n-electron ground state of the Friedel Hamiltonian (consisting of an electron band and a d resonance) can be exactly expressed as the sum of two Slater states

$$\Psi_{\mathrm{Fr}}=Aa_0^{\dagger}\prod_{i=1}^{n-1}a_i^{\dagger}\Phi_0+Bd^{\dagger}\prod_{i=1}^{n-1}a_i^{\dagger}\Phi_0, \tag{2}$$

where $a_0^{\dagger}$ is an artificial Friedel resonance state which determines uniquely the full orthonormal basis $\{a_i^{\dagger}\}$. An extension of this ground state to the Friedel-Anderson and Kondo impurity yields good numerical results. Recently this method was applied to calculate the Kondo polarization cloud for those impurities.[31] Therefore the author could not resist using the FAIR method to calculate the Friedel oscillations of a Kondo impurity. As in the paper by ABS I am treating the one-dimensional case. (The two- and three-dimensional treatments are essentially identical). Also the calculation is restricted to zero-impurity scattering (the same as in ABS's calculations).

The construction of the Wilson states is essentially the same in NRG and FAIR. One starts from an electron band with linear dispersion, as shown in Fig. 1. If one follows Wilson and measures the energy in units of the Fermi energy and the wave vector $\kappa=k/k_F$ in units of k_F then the dispersion is just

$$\varepsilon_\kappa=\kappa-1.$$

This band contains a macroscopic number of states φ_κ ($\approx 10^{23}$). Wilson subdivided the positive and negative half of the energy band by a factor λ. For example for $\lambda=2$ the negative band is divided into energy cells $\mathfrak{C}_0=(-1:-\frac{1}{2})$,

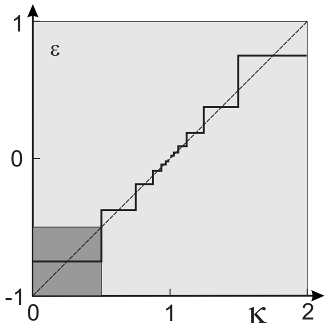

FIG. 1. The effective dispersion relation between energy ε and wave number κ in Wilson's Hamiltonian.

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$\mathfrak{C}_1=(-\frac{1}{2}:-\frac{1}{4}),\ldots,\ \mathfrak{C}_\nu=(\zeta_\nu:\zeta_{\nu+1})$, where $\zeta_\nu=-2^{-\nu}$. In each energy cell $\mathfrak{C}_\nu$ one has Z_ν states φ_κ with the energy $(\kappa-1)$. Assuming that each state $\varphi_\kappa(r)$ has the same interaction with the impurity then the states in the cell $\mathfrak{C}_\nu$ are combined to a new state $\psi_\nu(r)$,

$$\psi_\nu(r)=\frac{1}{\sqrt{Z_\nu}}\sum\nolimits_{\kappa\in\mathfrak{C}_\nu}\varphi_\kappa(r).$$

This state represents the full interaction of all states $\varphi_\kappa(r)$ in $\mathfrak{C}_\nu$ with the impurity (its interaction is enhanced by $\sqrt{Z_\nu}$). The sub-Hilbert space of $\mathfrak{C}_\nu$ contains $(Z_\nu-1)$ additional states,

$$\psi_\nu^l(r)=\frac{1}{\sqrt{Z_\nu}}\sum\nolimits_{\kappa_\mu\in\mathfrak{C}_\nu}\varphi_\kappa(r)\exp\left(i2\pi\frac{\mu l}{Z_\nu}\right)$$

with l and μ running from 0 to $(Z_\nu-1)$ (here ψ_ν^0 is identical to ψ_ν). The states with $l>0$ have no interaction with the impurity, but they have finite matrix elements $\langle\psi_\nu^l|H_0|\psi_\nu^{l'}\rangle$ with the band energy Hamiltonian H_0. These matrix elements are neglected in the NRG and the FAIR calculation. This is strictly speaking only correct when all the original states $\varphi_\kappa(r)$ in a given energy cell $\mathfrak{C}_\nu$ have the same energy. In Fig. 1 the energy–wave-vector diagram is shown. The dashed line gives the linear dispersion relation. The darkly shaded square marks the energy cell $\mathfrak{C}_0$. The thick zigzag line gives the dispersion for which the Wilson NRG would be exact.

In the one-dimensional case the wave functions φ_κ are cosine and sine functions (only the cosine states interact with the impurity). Since the energy ζ and the wave numbers κ are given in normalized units of ε_F and k_F, it is natural to measure distances also in reduced units. Throughout this paper lengths are measured in units of $\lambda_F/\mathbf{2}$, for example the distance from the impurity is denoted as $\xi=r/(\lambda_F/2)$. The Kondo length ξ_K is measured in the same units.

For the wave functions I use $\varphi_\kappa(\xi)=\sqrt{2/\Lambda}\cos(\pi\kappa\xi)$ in the range from $-\Lambda/2$ to $+\Lambda/2$. Here Λ is given by the size L of the one-dimensional box, $\Lambda=L/(\lambda_F/2)$. The number of states $\varphi_\kappa(\xi)$ in the energy cell $\mathfrak{C}_\nu$ is $(\zeta_{\nu+1}-\zeta_\nu)/(2/\Lambda)$.

This yields for the wave function of the Wilson state $\psi_\nu(\xi)$

$$\psi_\nu(\xi)=\frac{2}{\sqrt{(\zeta_{\nu+1}-\zeta_\nu)}}\frac{1}{\pi\xi}\sin\left(\pi\xi\frac{\zeta_{\nu+1}-\zeta_\nu}{2}\right)\times\cos\left[\pi\xi\left(1+\frac{\zeta_{\nu+1}+\zeta_\nu}{2}\right)\right]. \tag{3}$$

The exchange interaction is given by H_{sd},

$$H_{sd}=v_aJ\sum\nolimits_{\alpha,\beta}\Psi_\alpha^\dagger(0)\sigma_{\alpha,\beta}\Psi_\beta(0)\cdot\mathbf{S}, \tag{4}$$

where v_a is the atomic volume and J is the exchange interaction.

The FAIR method yields for the Kondo ground state

$$\Psi_K=[A_{s,d}a_{0+\uparrow}^\dagger d_\downarrow^\dagger+A_{d,s}d_\uparrow^\dagger a_{0-\downarrow}^\dagger]\overline{|0\rangle}+[A_{d,s}a_{0-\uparrow}^\dagger d_\downarrow^\dagger+A_{s,d}d_\uparrow^\dagger a_{0+\downarrow}^\dagger]\overline{\overline{|0\rangle}},$$

$$\overline{|0\rangle}=\prod_{i=1}^{n-1}a_{i+\uparrow}^\dagger\prod_{j=1}^{n-1}a_{j-\downarrow}^\dagger\Phi_0\ ,\quad \overline{\overline{|0\rangle}}=\prod_{i=1}^{n-1}a_{i-\uparrow}^\dagger\prod_{j=1}^{n-1}a_{j+\downarrow}^\dagger\Phi_0.$$

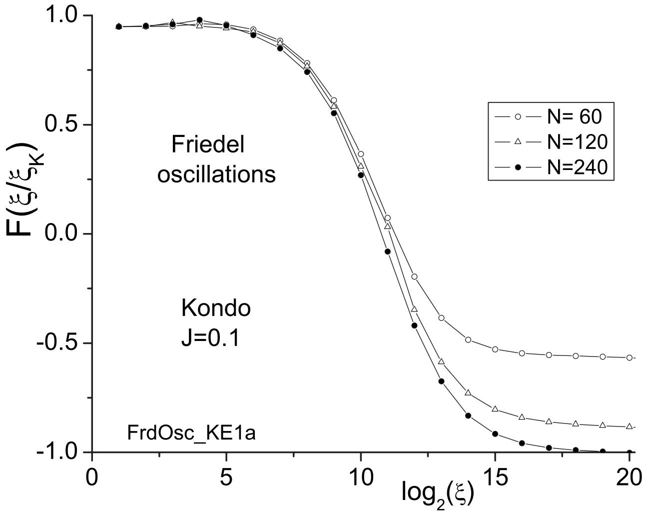

FIG. 2. The numerical result for the function $F(\xi/\xi_K)$ in Eq. (1) for different ratios of neighboring energies ζ_ν. For the number of Wilson states $N=60$ the ratio is $\lambda=2$, for $N=120$ it is $\lambda=\sqrt{2}$, and for $N=240$ it is $\lambda=\sqrt[4]{2}$.

The two FAIR states $a_{0+}^\dagger$ and $a_{0-}^\dagger$ are obtained by optimizing the ground-state energy (see for example Refs. 31 and 32). They have the form

$$a_{0\pm}^\dagger=\sum_\nu\alpha_{0\pm}^\nu c_\nu^\dagger,$$

where $c_\nu^\dagger$ are the creation operators of the Wilson states ψ_ν. (These two states are maximally coupled to the impurity.) The FAIR states $a_{0\pm}^\dagger$ determine uniquely the two bases $\{a_{i\pm}^\dagger\}$. The total charge density of the ground state Ψ_K can be calculated from the ground state with the help of the individual wave functions of the Wilson states.

To calculate the charge density of the Kondo ground state one has to calculate the charge densities of all states $a_{i\pm}^\dagger$ for $0\leq i<N/2$ and add them according to the occupation of these states. This yields the main contribution. But there are, in addition, two interference terms which yield rather small contributions. The total charge density is then calculated at average distances from the impurity of $2,4,8,..2^l,\ldots 2^{20}$. This is done in intervals of two wavelengths ($\Delta\xi=2$ or $\Delta r=\lambda_F$) where a dense trace of the charge density as a function of ξ is calculated. For each trace the position of the charge minima and maxima is determined as well as the amplitude.

In Fig. 2 the numerical result for $F(\xi/\xi_K)$ is plotted. It is the amplitude of the first term in Eq. (1), i.e., $C_D\cos(2k_Fr-D\frac{\pi}{2})/r^D$ [which in one dimension is equal to $\sin(2\pi\xi)/(2\pi\xi)$]. The abscissa is the logarithm (base 2) of the average distance ξ from the impurities. [The change in sign of $F(\xi/\xi_K)$ corresponds to a jump in the phase by π.]

The top curve with open circles is for $N=60$ Wilson states with a ratio $\lambda=2$ between neighboring energies ξ_ν. It confirms the statement by ABS that these Wilson states are not well enough suited for the calculation of small charge fluctuations on a length scale of the Fermi wavelength.

To improve the calculation I tried a different path than ABS. In the FAIR method the two essential states are the FAIR states $a_{0+}^{\dagger}$ and $a_{0-}^{\dagger}$. When they are known one can easily construct the full orthonormal basis for each FAIR state (with the condition that $\langle a_i^{\dagger}\Phi_0|H_0|a_j^{\dagger}\Phi_0\rangle=0$ for $i,j>0$). This is a trivial calculation with negligible computer time. Each $a_0^{\dagger}$ is composed of Wilson states

$$a_0=\sum_{\nu=0}^{N-1}\alpha_0^{\nu}c_{\nu}^{\dagger},$$

where $c_{\nu}^{\dagger}$ is the creation operator of the Wilson state ψ_{ν}. The square $|\alpha_0^{\nu}|^2$ gives the occupation or contribution of the state $c_{\nu}^{\dagger}$ or ψ_{ν} to $a_0^{\dagger}$. Since the state ψ_{ν} is constructed from the original states φ_k the ratio of $|\alpha_0^{\nu}|^2$ divided by width of the energy cell, i.e., $p_{\nu}=|\alpha_0^{\nu}|^2/(\zeta_{\nu+1}-\zeta_{\nu})$ gives the relative contribution of the original states φ_{κ} to the FAIR state $a_0^{\dagger}$. This state density p_{ν} corresponds to a function $p(\zeta)$ with the condition $p(\zeta)=p_{\nu}$ for $\zeta_{\nu}<\zeta<\zeta_{\nu+1}$. The integral of $p(\zeta)$ over the energy is normalized,

$$\int_{-1}^{+1}p(\zeta)d\zeta=\sum_{\nu=0}^{N-1}\int_{\zeta_{\nu}}^{\zeta_{\nu+1}}\frac{|\alpha_0^{\nu}|^2}{(\zeta_{\nu+1}-\zeta_{\nu})}d\zeta=\sum_{\nu=0}^{N-1}|\alpha_0^{\nu}|^2=1.$$

For large N the state density $p(\zeta)$ shows a smooth dependence on the energy. [This is shown in Fig. 4 for the example of a Friedel resonance (see below).] Therefore one can extrapolate $p(\zeta)$ from a finite representation N and construct the FAIR state for twice the number of states. The most natural way to double the number of Wilson states is to set a new energy ratio $\zeta_{\nu}'/\zeta_{\nu+1}'=\lambda'=\sqrt{\lambda}$. In this way the FAIR states and their full bases are obtained for $N=120$ (with a new $\lambda=\sqrt{2}$). It turns out that the new solution for Ψ_K is better than the old one (for $N=60$) because its ground-state energy is lowered. The second curve in Fig. 2 (open triangles) shows the numerical result for the function $F(\xi/\xi_K)$. It clearly improves the result although it does not yet reach the value -1 for large ξ. A second doubling of N yields $N=240$ and $\lambda=\sqrt[4]{2}$. The ratio of the width of an energy cell divided by the average energy is given by $2(\lambda-1)/(\lambda+1)$. For the usual Wilson states with $\lambda=2$ this ratio is 2/3. After two additional splitting of the states this ratio becomes about 0.173. Now the energy states are much closer together. For $N=240$ the numerical result for $F(\xi/\xi_K)$ is shown in the bottom curve of Fig. 2. It finally shows the two limiting values of +1 at short distances and -1 at large distances, in agreement with the theoretical prediction.

Since the function $F(\xi/\xi_K)$ is a universal function a comparison of Kondo impurities with different Kondo energies is appropriate. ABS performed a large number of calculations. I want to show that the FAIR method yields the same universality. In the past we investigated Kondo impurities with different exchange interactions and, therefore, different Kondo energies.[32] Here, I consider the two examples with $J=0.1$ and $J=0.08$. One obtains the Kondo lengths from the corresponding Kondo energies $\varepsilon_K=2.35\times10^{-5}$ and 1.37×10^{-6}.

In Fig. 2 we plotted the amplitude of the first term in Eq. (1) to extract the function $F(\xi/\xi_K)$. Now we determine the actual amplitude $A(\xi/\xi_K)$ of the Friedel oscillation, which is given by

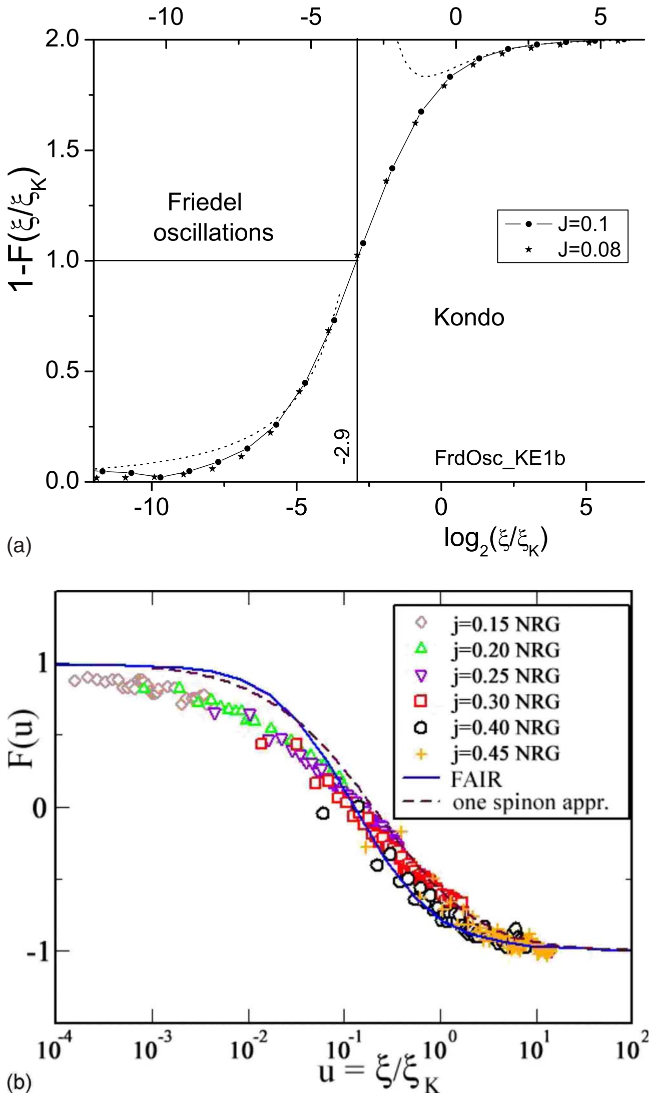

FIG. 3. (Color online) (a) The amplitude $[1-F(\xi/\xi_K)]$ of the Friedel oscillation for two different Kondo energies (this paper). (b) Reduction in the Friedel oscillation $F(\xi/\xi_K)$ is plotted versus ξ/ξ_K. The points are the numerical results by ABS; the full curve is the result of this paper.

$$\rho(\xi)-\rho_0=[F(\xi/\xi_K)-1]\frac{\cos\left(2\pi\xi-\dfrac{\pi}{2}\right)}{2\pi\xi}$$

$$=-A(\xi/\xi_K)\frac{\cos(2\pi\xi-\delta)}{2\pi\xi}.$$

In Fig. 3(a) this amplitude $A(\xi/\xi_K)=[1-F(\xi/\xi_K)]$ is plotted for the two different Kondo energies as a function of $\log_2(\xi/\xi_K)$. Since the abscissa has a logarithmic scale the curves are just shifted by $\log_2(\xi_K)$. Although the Kondo energies differ by roughly a factor of 5 the two curves are essentially identical. Therefore this calculation confirms that the amplitude of the Friedel oscillation is universal (for the symmetric case and a linear dispersion relation). The numerical calculation yields a phase shift of $\pi/2$ for distances larger than two Fermi wavelengths. For most of the region $(6 \le \log_2(\xi/\xi_K) \le 16)$ the relative deviation is less than 10^{-3}.

ABS gave two asymptotic functions for $\xi \ll \xi_K$ and $\xi \gg \xi_K$,

$$F(\xi/\xi_K) \rightarrow 1 - 3\pi^2/[8 \ln^2(\xi_K/\xi)]$$

for $\xi \ll \xi_K$ and

$$F(\xi/\xi_K) \rightarrow -1 + \pi w \xi_K/(4\xi) - 3(\pi W)^2 \xi_K^2/(32\xi^2)$$

for $\xi \gg \xi_K$, where $w \approx 0.4128$. These functions, which are shown as dotted curves in Fig. 3(a), have been shifted by 0.5 to the left (see upper scale). This means that I use a slightly different definition of the Kondo energy than ABS, which yields a different Kondo length. The ratio between our Kondo energies is $2^{0.5} \approx 1.4$. This is not surprising because ABS used Wilson's definition, which requires the NRG calculation, whereas we define the Kondo energy as the energy difference between triplet and singlet state.[32]

Figure 3(b) shows a comparison of the results of this paper and of ABS for the function $F(\xi/\xi_K)$. The full (blue) curve represents the data of this work, while the different points represent the numerical data of ABS for different interaction strengths. The explicit form of $F(\xi/\xi_K)$ is not known.

It is worthwhile mentioning that in my calculation the Kondo ground state is calculated once. From this ground state one obtains the Friedel oscillation for all distances ξ. ABS had to perform a new NRG calculation for each individual distance ξ (which actually represents states with slightly different ground-state energies).

One essential step in calculating the Friedel charge oscillations was the repeated doubling of the number of Wilson states. This was possible because the compositions of the FAIR states $a_{0+}^{\dagger}$ and $a_{0-}^{\dagger}$ are essentially given by the state-density functions $p_+(\zeta)$ and $p_-(\zeta)$. This shall be demonstrated for the FAIR state of a Friedel (resonance) impurity.

We take the Wilson electron band ranging from $(-1:+1)$ with constant density of states (equal to 1/2) and a d resonance at the Fermi energy $(E_d=0)$ with an s-d matrix element $|V_{sd}|^2=0.1$. The ground state is given in Eq. (2) with the FAIR state $a_0^{\dagger}$.

In Fig. 4 the values $p_\nu=|a_0^\nu|^2/(\zeta_{\nu+1}-\zeta_\nu)$ are plotted at the discrete energies $(\zeta_{\nu+1}+\zeta_\nu)/2$. The full circles are the values for $N=24$ and $\lambda=2$. Only a small fraction of the whole energy band is included in the figure to show an optimal section. The full triangles show the values for $N=48$ and $\lambda=\sqrt{2}$, while the stars represent the values of p_ν for $N=96$ and $\lambda=\sqrt[4]{2}$. For each N the optimal ground state has been derived. One recognizes that the points follow indeed a common function $p(\zeta)$. This justifies the doubling of the Wilson states since the new p_ν values can be obtained by interpolation and extrapolation. This yields the composition of the new FAIR state after the doubling of the number of Wilson states N.

As an afterthought of this consideration I calculated the Friedel oscillation for Friedel impurities with the d-resonance energy at the Fermi level, $E_d=0$, and very small resonance width $\Delta=\pi|V_{sd}|^2\rho$, where $\rho=1/2$ represents the density of states for the Wilson spectrum. By using rather small values for $|V_{sd}|^2=0.5\times10^{-4}$, 1.0×10^{-4}, and 2.0×10^{-4} one can evaluate the amplitude of the Friedel oscillations as a function of ξ.

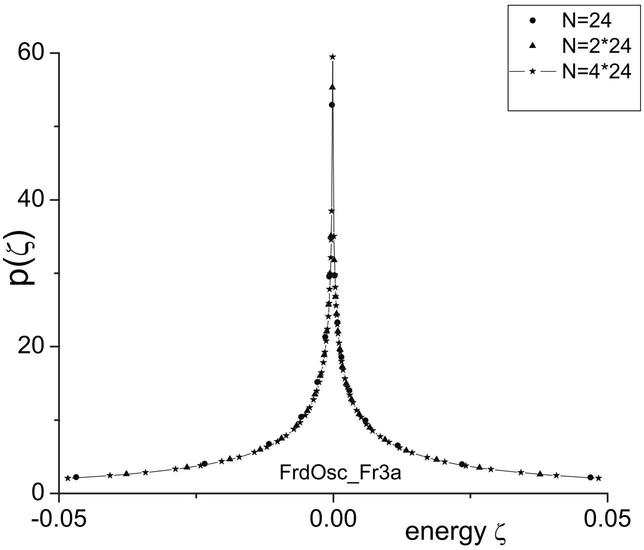

FIG. 4. The function $p(\zeta) \approx |\alpha_0^\nu|^2/(\zeta_{\nu+1}-\zeta_\nu)$ for $N=24,48,96$ with $\lambda=2,\sqrt{2}$ and $\sqrt[4]{2}$.

The numerical calculation yields a charge oscillation $\Delta\rho_{\mathrm{Fr}}=A_{\mathrm{Fr}}(\xi)\cos(2\pi\xi-\delta_{\mathrm{Fr}})/(2\pi\xi)$. The phase shift δ_{Fr} in the range $3 \le \log_2 \xi \le 19$ is equal to $\pi/2$ within 1% accuracy. For distances shorter than the Friedel coherence length $(\xi_{\mathrm{Fr}} \approx 2/|\pi V_{sd}|^2)$ the amplitude is strongly suppressed. The amplitude is also universal since the three curves in Fig. 5 would perfectly coincide if plotted as a function of (ξ/ξ_{Fr}). This behavior is quite analogous to the Friedel oscillations of a Kondo impurity. However, the functional dependence and the long-distance amplitude differ.

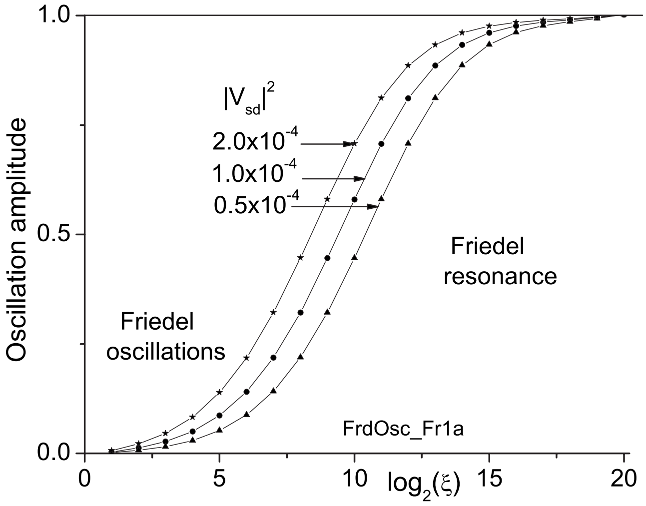

FIG. 5. The amplitude of the Friedel oscillation for Friedel impurities with s-d hopping matrix elements of $|V_{sd}|^2=2\times10^{-4}$, 1×10^{-4} and 0.5×10^{-4}. The Friedel oscillations develop only for distances larger than the Friedel length ξ_{Fr}.

To conclude, the goal of this paper has been to reproduce ABS result for the Friedel oscillations of a Kondo impurity with the FAIR method. This is a rather delicate problem because electron densities have to be calculated on a spatial scale much smaller than the Fermi wavelength λ_F over distances of up to $10^6\lambda_F$ with a relative accuracy of λ_F/r, i.e., 10^{-6} or better. The FAIR calculations confirm that the Friedel oscillations are strongly suppressed within a distance of the order of a tenth of the Kondo length.

The author is very much obliged to L. Borda who provided his original data and combined them with the data of this work in Fig. 3(b).

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*bergmann@usc.edu

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