On the Localization of Heavy Particles in Metals.

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Abstract

It has been conjectured\textsuperscript{1,2} that an impurity with charge $Z \geq 2$ can be localized due to its interaction with electrons in a metal. The simplest case is an impurity free to move between only two sites, which interacts locally with $s$-wave electrons. For $Z \geq 2$ the hopping of the impurity is formally irrelevant and this has been argued to lead to localization. In this paper it is shown that other processes, in particular joint hopping of the impurity and one or more electrons between the sites, play an important role and have not been treated properly in the literature. Being relevant in a renormalization group sense, even when $Z \geq 2$, these terms lead to delocalization of the impurity. Using bosonization, it is shown how these processes are generated from marginal operators that are usually neglected and the dangers of ignoring marginal or irrelevant operators are discussed in detail. Questions about implications for the more general situation of many sites to which the impurity can hop, are also considered.
I. INTRODUCTION

A very interesting but subtle problem for the past quarter century has been the low temperature (T) behavior of a heavy particle interacting with the electronic excitations in a metal. The subtleties arise from the competition between the tunneling of the heavy particle, which tends to delocalize it, and the inability of the electronic degrees of freedom to adjust to the potential of the moving particle, which tends to localize it. This difficulty is manifested in the orthogonality between the electronic ground states with the impurity located at two different points in space. This phenomenon, Anderson’s orthogonality catastrophe, is due to the fact that the two ground states differ by a very large number of very small energy particle-hole excitations. This infinity of excitations is related to the fact that the impurity at two different points in space creates Friedel oscillations in the electronic charge density of the metal which, due to a difference in the phase of the oscillations, differ from each other at arbitrary distances, implying particle-hole deformations at arbitrarily low energies.

In the limit of weak interactions between the heavy particle and the electrons the primary effect of the coupling to the electrons is to induce a frictional force on the otherwise free tunneling motion of the particle — although the dynamic properties of the impurity at low temperatures are only partially understood. In the opposite limit of strong interactions, it has been argued that the particle will be strictly localized. More specifically, it has been claimed that a charged particle with charge $Ze \geq 2e$ tunneling between symmetric positions that are well separated spatially will localize around one of the sites due to the interaction of the particle with $s$-wave electrons.

In this paper we will argue that a heavy particle interacting with the electrons via a small number of channels (less than or equal to four) cannot be localized by the interaction because of subtle effects that have not been treated fully in previous work. We will primarily focus on the simplest case in which the particle can tunnel between only two sites that are related by symmetry. This two site problem is related to the Kondo problem although there are important differences which have often been ignored in the literature. We primarily
assume local, screened, s-wave, spin independent interactions between the particle and the
electronic degrees of freedom. Due to the spin independence of the interaction we can then
neglect any possible spin of the heavy particle and treat the opposite spin electron species
independently.

At the end of the paper we will discuss the generalization of the problem due to the
presence of three or more sites to which the particle can hop, and also the potential relevance
of more angular momentum channels. We will argue that our results suggest the correct
behavior for the extended system of a particle in a periodic metal, and also have implications
for the sharpness of X-ray edge singularities in systems with mobile deep holes and other
related problems. The purpose of this paper is partially pedagogical, thus we work through
some parts in substantial detail, in particular pointing out the dangers that lurk within
many of the standard tricks, especially bosonization.

A. Outline

In the remainder of this Introduction we motivate the form of the Hamiltonian with which
we will primarily work and explain qualitatively the effects of the orthogonality catastrophe
on the motion of the particle as well as the effects that make it difficult to localize. The rest
of the paper is organized as follows: In the next section (II) we motivate and introduce the
standard and very useful method to perform the calculations, i.e. bosonization. The model
is introduced in the usual fermion representation of electrons which is then mapped into
bosons. In section III a path integral representation of the partition function is formulated
and brought into a Coulomb gas representation. Renormalization group flow equations
are derived and analyzed. In this way the results that were discussed qualitatively in the
Introduction are put on a firm footing. Subsequently in Section IV, the results, as well
as possible generalizations and complications, are discussed. Finally in Appendix A the
Coulomb gas representation of the partition function is rederived from the original fermion
representation and in Appendix B the two site problem is analyzed in the absence of any
symmetries other than the equivalence of the two sites.

B. Physical Picture

The Hamiltonian of the impurity–electron system has three important terms: the non-interacting electron part \( H_o \), the hopping of the heavy particle between the two sites and the interaction term \( U \). Thus:

\[
H = H_o + \Delta_o (d_1^+d_2 + d_2^+d_1) + U
\]

where \( d_1^+, d_2^+ \) are the creation operators of the impurity at sites 1, 2 and \( \Delta_o \) is the bare hopping matrix element of the impurity between the sites. We will generally neglect any asymmetry between the two sites. The interaction \( U \) will involve terms of the form \( d_1^+d_1c_n^+c_{n'} \) and \( d_2^+d_2c_n^+c_{n'} \) where \( c_n^+ \) are the creation operators of the electronic degrees of freedom. However, due to the assumed local nature of the potential we can rediagonalize the degrees of freedom of the electrons and be left with only two electronic degrees of freedom for each energy that are just composed of those wavefunctions which do not vanish at the two sites. Thus the potential \( U \) can be put in a form in which it involves two electronic states — albeit not free electron eigenstates — while all others decouple from the impurity. We can thus write the most general form for \( U \) in the following symmetric way:

\[
U = (d_1^+d_1 + d_2^+d_2)[V_1(c_1^+c_1 + c_2^+c_2) + V_2(c_1^+c_2 + c_2^+c_1)] \\
+ (d_1^+d_1 - d_2^+d_2)[V_3(c_1^+c_1 - c_2^+c_2) + iV_4(c_1^+c_2 - c_2^+c_1)]
\]

with matrix elements \( V_i \) to be determined. The interchange symmetry 1 \( \leftrightarrow \) 2 is manifest in \( U \). We have picked a basis for the electrons \( c_i, i = 1, 2 \) so that in the limit that \( R \), the distance between the two sites, tends to infinity, the \( c_i \)'s tend to the local s-wave annihilation operators at the two sites. As a result we expect \( V_2, V_4 \to 0 \) and \( V_3 \to V_1 \) as \( R \to \infty \). This will be seen explicitly later. Because there is only one heavy particle it is convenient to express \( U \) in form of Eq.(2) since \( d_1^+d_1 + d_2^+d_2 = 1 \). Therefore only \( V_3 \) and \( V_4 \) couple the
impurity to the electrons. One can see that the four terms in Eq. (2) are the only ones possible, due to the $1 \leftrightarrow 2$ interchange symmetry of $U$. From these four terms, by choosing the basis $c_i$ appropriately, one can make one term vanish since there are many ways we can choose normalized states that all tend to the local wavefunctions of the two sites as $R \to \infty$.

The freedom of choice of states is related to a gauge symmetry. If the system is time reversal invariant, to which we primarily restrict consideration, then a gauge can be chosen to make the Hamiltonian real and hence eliminate $V_4$. Note that, more generally, even in the absence of time reversal invariance $V_4$ could be eliminated formally at this point. But other operators would appear in the more detailed analysis which cannot be eliminated. Although we will not analyze these operators in detail, we will argue why they will not affect our main results.

Thus $H$ can be written as:

$$H = H_o + \Delta_o(d_1^+d_2 + d_2^+d_1) + V_1(c_1^+c_1 + c_2^+c_2)$$

$$+ V_2(c_1^+c_2 + c_2^+c_1) + V_3(d_1^+d_1 - d_2^+d_2)(c_1^+c_1 - c_2^+c_2)$$

(3)

using $d_1^+d_1 + d_2^+d_2 = 1$. In the next section we will explicitly derive this form and evaluate the $V_i$'s. In the standard manner, one can treat the relevant electronic degrees of freedom that comprise $c_1$ and $c_2$ as essentially one dimensional with the magnitude of $k$ playing the role of a one dimensional wavevector.

Let us now try to understand the effects of the potential on the motion of the particle. To start, we consider the simple limit with $R$ large so that the $V_2$ term which couples the two channels vanishes and $V_1 = V_3$. Thus we are left with two independent channels, $c_1$ and $c_2$, that interact locally with the impurity. Channel 1 electrons interact with the impurity when it is on site 1, ($d_1^+d_1 = 1$) with interaction strength $V_1$ and do not interact when the impurity is on site 2, ($d_2^+d_2 = 1$). The opposite holds for channel 2. The important physics arises from the effect of the impurity at a given site on the electrons. If, for example, the potential is attractive, then the impurity tends to attract electrons towards it in order to screen its presence. Thus when the impurity is on site 1, it will tend to shift electrons of
channel 1 towards site 1. A rather naive picture of this shifting is the induction of charge in a metal close to a positively charged object in order to screen the electric field in the bulk of the metal. The induced charge comes from the outer boundaries of the metal and thus from arbitrarily far away.

A better interpretation is in terms of the wavefunctions of the electrons. Due to the existence of the attractive potential the wavefunctions far away from the potential center look just like the non-interacting ones except for a phase shift. This implies that some extra charge density has moved in from far away to screen the impurity. Indeed Friedel’s sum rule relates the phase shifts $\delta_\ell$ at the Fermi level to the charge, $Ze$, that is needed to screen a charged impurity,

$$Z = 2 \sum_\ell (2\ell + 1) \frac{\delta_\ell(k_F)}{\pi}$$

where the sum is over the angular momenta channels $\ell$; the sum over the spins yields the factor of 2. Thus we can interpret

$$n_\ell = \frac{\delta_\ell}{\pi}$$

as the number of electrons per channel that need to be shifted close to the given site in order to screen the potential. For the present discussion we will assume that only one angular momentum channel $\ell = 0$ plays a role.

Now since the impurity can move from site to site, in order to understand the effect of the interaction on the dynamics of the impurity we need to know the time dependent amplitude of a process in which the impurity hops away from a given site for a certain amount of time $t$ before it hops back to the previous site. When $t$ is long enough we can view this process in the following simple way: until time $t = 0$ the impurity has been at, say, site 1. At $t = 0$ the particle tunnels to site 2 where it remains for a time $t$ before tunnelling back to 1. When the particle hops away from site 1, there are $n = \delta/\pi$ extra electrons of each spin within a screening distance from site 1 that will move away as the system evolves to its new ground state. Similarly there are $n$ extra holes of each spin near site 2. With the sites far apart, the evolution of the s-wave electrons around each site are essentially independent.
Following Schotte and Schotte\textsuperscript{8} we can get a semi-quantitative understanding of the amplitude of the hopping process by considering $\delta/\pi = n$ with $n$ an integer. Between time zero and $t$, the $n$ extra $s$-wave spin-up electrons in channel 1 propagate as in absence of the potential that earlier kept them near site 1. To estimate the amplitude of the total process, we need to find the matrix element between this evolved state at time $t$ and the ground state with the particle back at site 1, i.e. the initial state at time zero. Since the radial distance from site 1 of the $s$-wave electrons can be treated as essentially a one dimensional coordinate, we can obtain the $t$-dependence of this process, roughly, by creating the $n$ electrons at distances $a$, $2a$, . . . , $na$ from site 2 with $na$ of the order of the screening distance. (A better approximation would involve an integral over the positions of the extra electrons with a weighting factor related to the wave functions in the presence of the impurity at site 1; but this will only modify our crude estimate by a multiplicative prefactor.) We thus need to compute the amplitude\textsuperscript{2}

$$A_n(t) = \langle 0 | c(a, t) \cdots c((n-1)a, t)c(na, t)c^+(na, 0) \cdots c^+(2a, 0)c^+(a, 0)|0 \rangle \quad (6)$$

in a one dimensional system with no potential, with all the electrons moving at the Fermi velocity $v_F$ in the same direction. At long times, the antisymmetry of Eq.(6) under exchange of any two space variables fixes the form of $A_n$. When $t \gg \tau_c = a/v_F$, the sum over all possible Wick pairings in Eq.(6) with the one dimensional long time propagator $G_o \propto \left[ i(t-x/v_F) \right]^{-1}$ yields

$$A_n \propto \det[t + (j-i)\tau_c]^{-1}. \quad (7)$$

The determinant is of the $n \times n$ matrix with $i$ and $j$ subscripts. By use of the properties of determinants, this can be shown to yield:

$$A_n \propto \prod_{i<j} [(i-j)\tau_c]^2 \prod_{i,j} [(j-i)\tau_c + t]^{-1} \sim t^{-n^2} \quad (8)$$

for long $t \ll \tau_c$. The same result will obtain for the down spin electrons as well as for the $s$-wave holes around site 2. Thus the amplitude for the full double-hop process will be
$A \propto t^{-4n^2}$. In general, with different spin, angular momentum and site channels, $\gamma$, with $n_\gamma$ electrons moved in channel $\gamma$, the amplitude will be $A \propto t^{-\sum_\gamma n_\gamma^2}$. Later we will see that the general result for far away sites is to simply replace $n_\gamma$ by an appropriate phase shift $n_\gamma = \delta_\gamma/\pi$.

It is convenient to define an exponent $\alpha_o$

$$\alpha_o = \frac{1}{2} \sum_\gamma n_\gamma^2$$

so that the amplitude of the double-hop process will be, including dependence on the bare hopping amplitude $\Delta_o$,

$$A(t) \sim \Delta_o^2 t^{-2\alpha_o}.$$ (10)

If the sites are not far apart, or the system is not rotationally invariant, there will nevertheless still be quantities analogous to $n_\gamma$, with the interpretation as charge moved in a “channel”, such that Eq.(10) obtains, even though the phase shifts no longer have any meaning, see Appendix B.

In order to understand the dynamics in the presence of the coupling to the electrons, we make the standard argument, with the Ansatz that in equilibrium, the heavy particle hops back and forth at a rate $\Delta \bar{=} \bar{=}$. The amplitude for this hopping can thus be guessed to be the square root of the double-hop amplitude $A(t \sim 1/\Delta)$ since the particle will spend time of order $1/\Delta$ at each site before hopping back. Thus the amplitude will be of order $A(t \sim 1/\Delta)$ for each pair of hops, so that, from Eq.(10) we have

$$\Delta^2 \sim \Delta_o^2 \Delta^{2\alpha_o}.$$ (11)

This has the following solution:

$$\Delta = \begin{cases} 
0 & \text{for } \alpha_o > 1 \\
c \Delta_o^{\frac{1}{1-\alpha_o}} & \text{for } \alpha_o < 1 
\end{cases}$$ (12)

We thus see that for $\alpha_o > 1$ the real hopping process will not take place and we are thereby lead to the conclusion that the impurity will localize on the site on which it started undergoing only short virtual hops back and forth to the other site. With only $s$-wave scattering
off the impurity Friedel’s sum rule yields $Z = 2\delta_o/\pi$ with $\delta_o$ the s-wave channel phase shift for the potential $V = V_1 = V_3$ and the factor of 2 coming from the two spin species. As a result, for well separated sites,

$$\alpha_o = 2(\frac{\delta_o}{\pi})^2 = \frac{Z^2}{2} > 1$$

obtaining the inequality if $Z \geq 2$, so that a charge two particle will be localized although a charge one particle will not be.

This is the conclusion that has been reached, by this argument and more sophisticated versions of it, by a number of authors[1,2,5,9]. It seems widely accepted - along with the extension of the result to the localization of a particle moving on a lattice of sites. Note, furthermore that if there were more angular momentum channels present with phase shifts of both signs, it should be possible, by the above argument, to localize even a neutral or charge one particle provided the phase shifts are in the regime in which the exponent $\alpha_o > 1$. The main point of this paper is that these conclusions are not justified. Although we will see that it still appears to be possible to localize a particle, this cannot be achieved by just s-wave scattering for any charge, and in fact requires at least three angular momentum channels to have substantial coupling (so that s and the three p channels may be sufficient).

We will see that the approximation of neglecting the $V_2$ coupling is very dangerous. In contrast, relaxing the approximation of $V_3 = V_1$ will not change much and the relevant phase shifts will be those associated with $V_3$. However the crucial $V_2$ term changes the symmetry of the problem: The Hamiltonian in Eq.(3) with $V_2 = 0$ and the $c_1$ and $c_2$ electrons uncoupled, has the continuous extra gauge symmetry

$$c_1 \rightarrow c_1$$
$$c_2 \rightarrow e^{i\phi}c_2$$

that is broken by $V_2$. The $V_2$ term mixes the two channels around the two sites (although the mixing will be weak for large intersite separations). This term allows processes in which one or more electrons near one site transform to electrons near the other. We shall see that these yield processes in which the impurity hops from one site to the other simultaneously
with a number of electrons moving from one site to the other. In terms of the interpretation of the exponent for the time dependence of a process as a square of the charge transferred (such as Eq(9)) we see that the exponent for a process in which the impurity and a hole of each spin hop together will be

$$\alpha_1 = 2(n_o - 1)^2. \quad (15)$$

This process is illustrated in Figure 1. In general the process in which the impurity moves from site 1 to 2 at the same time as m holes of each spin transfer from site 1 to site 2, will have an orthogonality exponent

$$\alpha_m = 2(n_o - m)^2. \quad (16)$$

Thus using the self-consistent argument for localization outlined above, we conclude that in the case of s-wave scattering with $n_o = Z/2$, regardless of the charge of the impurity, it will never become localized because there will always be a process with m pairs of holes with m such that $|\frac{Z}{2} - m| < \frac{1}{2}$ for which

$$\alpha_m = 2(n_o - m)^2 = 2 \left( \frac{Z}{2} - m \right)^2 < \frac{1}{2}. \quad (17)$$

This process will yield a non-zero hopping rate and will delocalize the particle.

Physically, a process in which a number of electrons hop as well as the impurity, schematically shown in Fig.1, means that in a sense, less of the screening cloud hops back and forth that one would expect from the behavior of the ground state of the static impurity. The combined process can be thought of as the tunnelling back and forth not between the static-impurity ground states, but between excited states, with the extra action associated with this combined process more than compensated for by its larger matrix element (since it has a smaller orthogonality exponent). The process with the least action overall will dominate the impurity hopping.

We shall see that this effect can easily be missed, and indeed it seems to have been missed in the literature\textsuperscript{1,2,7}, even though a number of authors have considered “electron assisted
tunnelling” processes in which the heavy particle hops simultaneously with one electron (another process that can occur). This process was also introduced in a spinless version of the X-ray edge problem in a recent numerical work by Libero and Oliveira. The main theoretical difficulty is that in certain representations (e.g., choices of fields to bosonize) the important extra impurity-electron hopping terms are generated, under renormalization, from marginal terms (such as $V_2$) which are themselves only generated from irrelevant operators. As happens all too often, irrelevant operators cannot just be cavalierly thrown away!

II. MODEL

In this Section we introduce a simple model with short-range interactions, show how it can be cast in the form of Eq(3) and then begin to analyze it by bosonization of the electron fields, pointing out some of the pitfalls.

A. Definitions

We start with the Hamiltonian

$$H = H_o + \sum_{\sigma = \pm} U_\sigma + \Delta_\sigma (d_1^+ d_2 + d_2^+ d_1)$$

where the free electron Hamiltonian $H_o$ can be written as

$$H_o = \int_k \varepsilon_k c_{k\sigma}^+ c_{k\sigma}$$

with $\int_k = \int \frac{d^3k}{(2\pi)^3}$ and with $c_{k\sigma}^+$ being the creation operators of electrons at momentum $k$, spin $\sigma$ and energy $\varepsilon_k$. Finally $U_\sigma$ is a short-range interaction between electrons and the impurity

$$U_\sigma = V \int_k \int_{k'} e^{-i(k-k') \cdot r_1} c_{k\sigma}^+ c_{k'\sigma} d_1^+ d_1 + V \int_k \int_{k'} e^{-i(k-k') \cdot r_2} c_{k\sigma}^+ c_{k'\sigma} d_2^+ d_2$$

with $V$ the interaction strength and $r_i$ the position of the $i$-th site. If we put the center of coordinates between the two sites then we can set $r_1 = -\frac{R}{2}$ and $r_2 = \frac{R}{2}$ with $R = r_1 - r_2$. 
In order to eliminate the unimportant degrees of freedom that are decoupled from the impurity we integrate over the $k$–solid angles and are left with a set of effectively one-dimensional degrees of freedom. Neglecting for now the spin index $\sigma$, we define $\hat{c}_\pm k$ via:

$$\int \frac{dk}{2\pi} \hat{c}_\pm k = \int \frac{d^3k}{(2\pi)^3} e^{\pm i k \cdot \mathbf{R}} c_k = \int \frac{dk}{2\pi} \left[ \int \frac{k^2 d\Omega_k}{2} e^{\pm i k \cdot \mathbf{R}} c_k \right]$$

with $d\Omega_k$ being the solid angle element in $k$-space. But now these one-dimensional Fermi operators are not properly orthogonal. This is manifested by nonvanishing anticommutation relations ($\{\hat{c}_+ k, \hat{c}_- k\} \neq 0$). An orthonormal set of states can be made from these that are even and odd under the interchange of the two sites:

$$c_{ek}^+ = \frac{1}{\sqrt{N_e}} (\hat{c}_{+k}^+ + \hat{c}_{-k}^+)$$
$$c_{ok}^+ = \frac{1}{\sqrt{N_o}} (\hat{c}_{+k}^+ - \hat{c}_{-k}^+)$$

where the subscripts e,o denote, respectively even and odd while the normalization constants $N_{e,o}$

$$N_{e,o}(k) = \frac{2k^2}{\pi} \left( 1 \pm \sin \frac{kR}{kR} \right)$$

are picked so that $c_{ek}$ and $c_{ok}$ satisfy one-dimensional anticommutation relations:

$$\{c_{ek}^+, c_{ek'}^+\} = 2\pi \delta(k - k')$$ etc.

From these states we can obtain linear combinations

$$c_{1k}^+ = \frac{c_{ek}^+ + c_{ok}^+}{\sqrt{2}}$$
$$c_{2k}^+ = \frac{c_{ek}^+ - c_{ok}^+}{\sqrt{2}}$$

which transform into each other under interchange of the two sites. It is interesting to note that $c_{1,2}^+$ are the only orthonormal states that have this symmetry for arbitrary $kR$. To see this one could basically define the most general pair of orthonormal states with interchange symmetry:
\[ c_{1k}^+ = \alpha \hat{c}_{+k}^+ + \beta e^{i\theta} \hat{c}_{-k}^+ \]
\[ c_{2k}^+ = \beta e^{i\theta} \hat{c}_{+k}^+ + \alpha \hat{c}_{-k}^+ \]  \tag{26}

with \( k \)-dependent \( \alpha, \beta, \theta \). Eq\textsuperscript{(26)} is well defined only if \( |\cos \theta| > \left| \frac{\sin kR}{kR} \right| \). Thus for small \( kR \) we must set \( \theta \approx 0 \) while for large \( kR \) the two sites are decoupled and \( \theta \) can take almost any value; for \( \theta = 0 \) Eq\textsuperscript{(26)} becomes Eq\textsuperscript{(25)} with the use of Eq\textsuperscript{(22)}. Now we can invert Eq\textsuperscript{(26)} and using Eq\textsuperscript{(21)}, substitute into the potential \( U \) in Eq\textsuperscript{(20)}. Since the only values of \( k \) that play a significant role are \( k \approx k_F \) we can set \( \alpha, \beta \) (equivalently \( N_e, N_o \)) to a constant evaluated at \( k_F \). Thus using

\[ c_i^+ = \int \frac{dk}{2\pi} c_{ik}^+ \quad \text{with} \quad i = 1, 2 \]  \tag{27}

with the integral running over \( k \) in the neighborhood of \( k_F \) with an appropriate cutoff of order \( k_F \), we get an expression for the potential identical to Eq\textsuperscript{(2)}. Henceforth we will choose \( \theta = 0 \) for all \( k \) which yields \( V_4 = 0 \) in Eq\textsuperscript{(2)} thereby explicitly exhibiting the time-reversal invariance.

Furthermore we can obtain the other coefficients \( V_i \) in Eq\textsuperscript{(2)} starting from Eq\textsuperscript{(20)} by using the relation between the free electron density of states per spin at \( \varepsilon = \varepsilon_F, \rho_F \), with the Fermi momentum \( k_F \); after rescaling the Fermi velocity to be one, \( 2\pi^2 \rho_F = k_F^2 \). We then get:

\[ V_1 = \pi \rho_F V \]
\[ V_2 = \pi \rho_F V \frac{\sin k_F R}{k_F R} \]
\[ V_3 = \pi \rho_F V \sqrt{1 - \left( \frac{\sin k_F R}{k_F R} \right)^2} \]  \tag{28}

It is also instructive to write \( U \) using the even-odd states from Eq\textsuperscript{(22)}. Defining

\[ c_{e,o}^+ = \frac{c_1^+ \pm c_2^+}{\sqrt{2}} \]  \tag{29}

we obtain:

\[ U = V_1 \left( c_e^+ c_e + c_o^+ c_o \right) + V_2 \left( c_e^+ c_e - c_o^+ c_o \right) + V_3 \left( d_1^+ d_1 - d_2^+ d_2 \right) \left( c_e^+ c_o + c_o^+ c_e \right) \]  \tag{30}
Comparing Eq(30) with Eq(2) we see that (with \( V_4 = 0 \)) the non-interacting part of \( U \) is diagonal in the even-odd representation while the interacting part is diagonal in the \( c_{1,2} \) representation.

Finally, we make the standard change of variables for a two state system, i.e.

\[
d_+^+ d_2 - d_1^+ d_1 = \sigma_z \\
d_1^+ d_2 + d_2^+ d_1 = \sigma_x.
\]

In this representation the impurity in site 1 (2) is in state \((-\)) of the \( \sigma_z \) operator. Thus \( d_1^+ |0\rangle = |-\rangle \) while \( d_2^+ |0\rangle = |+\rangle \) where \( |0\rangle \) is the ground state of \( H_o \).

Summarizing, the Hamiltonian can be written as

\[
H = H_o + \Delta_o \sigma_x + U
\]

with

\[
U = V_1 \left( c_1^+ c_1 + c_2^+ c_2 \right) + V_2 \left( c_1^+ c_2 + c_2^+ c_1 \right) + V_3 \left( c_2^+ c_2 - c_1^+ c_1 \right) \sigma_z
\]

and with \( V_i \) given by Eq(28) and \( c_i \) given by Eq(25) (where \( i = 1, 2 \)) while

\[
H_o = \sum_{i=1,2} \int \frac{dk}{2\pi} \varepsilon_k c_{ik}^+ c_{ik}
\]

and

\[
\varepsilon_k = \frac{k^2}{2m} - \frac{k_F^2}{2m} \approx (k - k_F)
\]

with Fermi velocity set equal to unity.

The electrons that interact with the impurity are thus effectively two species of one-dimensional fermions moving only to the right, with those to the left of the origin corresponding to incoming electrons while those to the right of the origin corresponding to outgoing electrons.

At this point it is useful to pause and consider the symmetries of the effective Hamiltonian in Eq(32). There is a global \( U(1) \) gauge symmetry — of the electron phase — and a discrete
interchange symmetry $1 \leftrightarrow 2$. However note that in the absence of the $V_2$, there would be an extra gauge symmetry, that of Eq(14). Although in some formulations it appears that $V_2$ can be made to disappear, this is potentially dangerous as $V_2$ breaks the artificial extra gauge symmetry and the formally irrelevant operators which break the symmetry should thus be retained.

It is instructive to see how the problem with trying to get rid of $V_2$ can be seen in the fermion representation; in Appendix B the analysis will be done in considerable detail using the boson representation introduced in the next sub-section. Using the even-odd representation of Eq(30), one can indeed rediagonalize the even-odd channels and absorb the $V_1, V_2$ terms into $H_o$. This leaves the long time Green’s functions of the even-odd channels unaffected but changes the short time behavior (see, for example, Nozières and De Dominicis). Thus

$$\langle c_e^+(\tau)c_e(0) \rangle \neq \langle c_o^+(\tau)c_o(0) \rangle$$

for $\tau$ small, of order the cutoff $\tau_c$. Performing perturbation theory in $V_3$ to second order we get a correction in $U$

$$\delta U \propto V_3^2 \left\{ c_e^+c_e \left( \langle c_o c_o^+ \rangle - \langle c_o^+ c_o \rangle \right) + c_o^+c_o \left( \langle c_e c_e^+ \rangle - \langle c_e^+ c_e \rangle \right) \right\}.$$  

In general, $\langle c^+ c \rangle \neq \langle c c^+ \rangle$ due to the nonlinear dispersion of fermions away from $k_F$, in particular particle-hole asymmetry. Thus, from Eq(36) we see that the asymmetry between the even-odd channels reappears in perturbation theory, due to the short time (high-energy) details. As a result we must retain the $V_2$ term in the Hamiltonian.

**B. Bosonization**

In order to proceed it is necessary to find a representation that focuses on the essential low energy parts of the problem. Then, even if the problem is not exactly solvable, one can at least hope to be able to understand the physics and predict the low energy behav-
ior. The most commonly used representations are boson representations of the pseudo-one dimensional fermions.

The basic strategy of bosonization is to try to mimic the low energy physics of the Fermi system, which can only be done exactly for a particularly simple system of exactly linear one-dimensional bands with a specific form of the cutoff. In more general situations, it is hoped (or, better, demonstrated!) that the high energy terms that are ignored — for example particle-hole excitations far from the Fermi surface — only serve to give finite renormalizations of the basic parameters of the dominant low energy operators in the Hamiltonian. High energy properties — for example the fermion anticommutation relations — are, ipso facto, only handled approximately. What is more important, but unfortunately sometimes forgotten, is that terms that are formally irrelevant at low energies can, either on their own, when combined with other terms, or under canonical transformations, produce relevant or marginal terms that affect the physics. As we shall see, this is the case for the present problem.

For now we will proceed in the conventional manner. Let us then start with the non-interacting Hamiltonian, \( H_o \). If we are primarily interested in energies close to \( \varepsilon_F \), we can extend the linear dispersion relation to all energies. Thus if we set the origin of \( k \) at \( k = k_F \) for convenience, we will get by Fourier transforming:

\[
H_o = \sum_{j=1,2} \int_{-\infty}^{\infty} dx \left[ \Psi_j^+(x) \left( -i \frac{\partial}{\partial x} \right) \Psi_j(x) \right]
\]

where \( x \) is the conjugate variable to \( k \) and \( \Psi_j(x) \) is the Fourier transform of \( c_{jk} \):

\[
\Psi_j(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} c_{jk} \quad j = 1, 2
\]

Note that there are only right moving fermions in the system since there is only one Fermi point, i.e. one \( k \)-value at which \( \epsilon_k = \epsilon_F \).

The operators at the impurity sites are given in terms of

\[
c_j = \int \frac{dk}{2\pi} c_{jk} = \Psi_j(0) \quad j = 1, 2
\]
which identifies $c_j$ as the $x = 0$ creation operator in the one dimensional picture. Roughly speaking, $\Psi_j(x)$ with $x < 0$ corresponds to incoming $s$-wave electrons around site $j$ while with $x > 0$, it corresponds to outgoing $s$-wave electrons. Thus the time reversal operator acting on $\Psi_j(x)$ will give:

$$\hat{T}\Psi_j(x) = \Psi_j(-x)$$  \hspace{1cm} (41)

since it transforms incoming to outgoing electrons and vice-versa.

At this point we can introduce the bosonic fields $\Phi_j(x)$ by:

$$\Psi_j^+(x) = \frac{1}{\sqrt{2\pi\tau_c}} e^{i\phi_j(x)}$$  \hspace{1cm} (42)

with $\tau_c^{-1} \propto k_F$ the characteristic cutoff frequency of the order the Fermi energy, and

$$\Phi_j(x) = \sqrt{\pi} \left[ \phi_j(x) - \int_{-\infty}^{x} \Pi_j(x')dx' \right]$$  \hspace{1cm} (43)

with $\phi_j$ and $\Pi_j$ satisfying appropriate commutation relations:

$$[\phi_j(x), \Pi_i(y)] = i\delta_{ij} \frac{\tau_c}{\pi \left( \tau_c^2 + (x-y)^2 \right)}$$  \hspace{1cm} (44)

In the continuum limit $\tau_c \to 0$, this commutation relation approaches $i\delta_{ij}\delta(x-y)$. From Eq(41) and Eq(42) it can be seen that $\Phi_j(x)$ transforms under time reversal as follows:

$$\hat{T}\Phi_j(x) = -\Phi_j(-x).$$  \hspace{1cm} (45)

Expanding $\phi_j(x)$ and $\Pi_j(x)$ in terms of their Fourier components,

$$\phi_j(x) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi\sqrt{2|\epsilon|}} \left[ \phi_j(\epsilon)e^{i\epsilon x} + \phi_j^+(\epsilon)e^{-i\epsilon x} \right] e^{-\frac{|\epsilon|\tau_c}{2}}$$

$$\Pi_j(x) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi\sqrt{2|\epsilon|}} \left[ -i\phi_j(\epsilon)e^{i\epsilon x} + i\phi_j^+(\epsilon)e^{-i\epsilon x} \right] e^{-\frac{|\epsilon|\tau_c}{2}}$$  \hspace{1cm} (46)

and inserting these expressions in Eq(43), $\Phi_j$ can be written as:

$$\Phi_j(x) = \int_{0}^{\infty} \frac{d\epsilon}{\sqrt{2\pi\epsilon}} \left[ \phi_j(\epsilon)e^{i\epsilon x} + \phi_j^+(\epsilon)e^{-i\epsilon x} \right] e^{-\frac{|\epsilon|\tau_c}{2}}$$  \hspace{1cm} (47)
which involves only the positive energy parts. Subsequently inserting Eq(47) in Eq(42) and then in Eq(38) the non-constant part of $H_o$ becomes

$$H_o = \sum_{j=1,2} \int_0^\infty \frac{d\epsilon}{2\pi} \phi_j^+(\epsilon) \phi_j(\epsilon) e^{-\epsilon \tau_c}$$

with

$$[\phi_i(\epsilon), \phi_j^+(\epsilon')] = \delta_{ij} 2\pi \delta(\epsilon - \epsilon')$$

Finally using the standard expression

$$\Psi_j^+(x) \Psi_j(x) = \frac{1}{2\pi} \frac{\partial \Phi_j(x)}{\partial x},$$

the potential $U$ is found to be:

$$U = \frac{V_1}{2\pi} \left[ \frac{\partial \Phi_1(0)}{\partial x} + \frac{\partial \Phi_2(0)}{\partial x} \right] + \frac{V_2}{\pi \tau_c} \cos[\Phi_1(0) + \Phi_2(0)] + \frac{V_3}{2\pi \sigma_z} \left[ \frac{\partial \Phi_2(0)}{\partial x} - \frac{\partial \Phi_1(0)}{\partial x} \right].$$

The form of $U$ may be simplified by introducing Bose fields corresponding to collective modes for excitations that are even, $\Phi_e(x)$, and odd, $\Phi_o(x)$, about the center of symmetry of the pair of sites:

$$\Phi_e = \frac{1}{\sqrt{2}} (\Phi_1 + \Phi_2)$$
$$\Phi_o = \frac{1}{\sqrt{2}} (\Phi_2 - \Phi_1)$$

The $\phi_{e,o}$ and $\Pi_{e,o}$ can be defined equivalently. In terms of the new variables $H_o$ remains in diagonal quadratic form (i.e. the indices $j = 1, 2$ in Eq(48) are replaced by $j' = e, o$), corresponding to free bosons and $U$ becomes

$$U = \frac{V_1}{\sqrt{2\pi}} \frac{\partial \Phi_e(0)}{\partial x} + \frac{V_2}{\pi \tau_c} \cos[\sqrt{2}\Phi_o(0)] + \frac{V_3}{\sqrt{2\pi} \sigma_z} \frac{\partial \Phi_o(0)}{\partial x}$$

The symmetries of the problem are manifest in Eq(53), $\Phi_e \rightarrow \Phi_e + c$ corresponding to the global gauge invariance, $\sigma_z \rightarrow -\sigma_z$ with $\Phi_o \rightarrow -\Phi_o$ corresponding to the interchange symmetry, and $\Phi_o \rightarrow \Phi_o + \pi \sqrt{2}$ corresponding to $c_j^+ \rightarrow -c_j^+$ for $j = 1, 2$. Note that the even mode is completely decoupled from the impurity in Eq(53) and will therefore not
play a role. Formally it can be eliminated by a unitary transformation $H \rightarrow \Lambda_e H \Lambda_e^{-1}$ with $
abla \Lambda_e = \exp[-i \frac{V}{2\pi} \Phi_e(0)]$; we perform this transformation and henceforth only consider the potential Eq(53) without the $V_1$ term.

In addition, Eq(53) also has the symmetry: $\Phi_{e,o} \rightarrow -\Phi_{e,o}$ and $x \rightarrow -x$ corresponding to time reversal invariance from Eq(43). If the system were not time reversal invariant, then one could have $V_4 \neq 0$. Indeed, the lowest order time reversal symmetry breaking term is $\sigma_z \sin \left[ \sqrt{2} \Phi_o(0) \right]$ which is exactly the $V_4$ term. However, we argued (above Eq(3)) that $V_4$ can always be chosen to be zero. But in the absence of time reversal invariance, such terms as $\frac{\partial \Phi_o(0)}{\partial x} \sin \left[ \sqrt{2} \Phi_o(0) \right]$ can also appear, essentially from nonlinear dispersion of the fermions away from $k_F$ and energy dependence of the scattering, that breaks the time reversal symmetry of the even or odd channels. Although these appear to be irrelevant, they cannot simply be eliminated because they generate a $\sigma_z \sin \left[ \sqrt{2} \Phi_o(0) \right]$ term after the unitary transformation of Eq(59) is performed. In order to eliminate such terms one has to pick a gauge or, equivalently a basis for the fermions (i.e. pick appropriate $\alpha, \beta, \theta$ in Eq(26)) which creates a $V_4$-term that exactly cancels the generated $\sigma_z \sin \left[ \sqrt{2} \Phi_o(0) \right]$ term. In effect, one would thus obtain a set of almost time-reversal invariant low energy excitations, and our main results would still obtain.

But danger lurks: even with full time reversal invariance similar terms to those discussed above will invalidate a related form of bosonization that we now discuss. It is tempting to find a way to get rid of the $V_2$ term by a different choice of bosonization. One way to do this is to start with $U$ in the form of Eq(30) and bosonize the fields $c_{ek}$ and $c_{ok}$. In this case one has to introduce the fields $\Psi'_e(x)$ and $\Psi'_o(x)$ in an analogous way to $\Psi_1(x)$ and $\Psi_2(x)$ in Eq(42):

$$
\Psi'_e(x) = \frac{1}{\sqrt{2\pi \tau_c}} e^{-i\Phi'_e(x)}
$$

$$
\Psi'_o(x) = \frac{1}{\sqrt{2\pi \tau_c}} e^{-i\Phi'_o(x)}
$$

with $\Phi'_{e,o}(x)$ different from $\Phi_{e,o}(x)$ in Eq(52). Subsequently by introducing linear combinations of these fields

$$
\Phi'_e(0) = \frac{1}{\sqrt{2\pi \tau_c}} e^{-i\Phi'_e(x)}
$$

with $\Phi'_{e,o}(x)$ different from $\Phi_{e,o}(x)$ in Eq(52). Subsequently by introducing linear combinations of these fields

$$
\Phi'_o(0) = \frac{1}{\sqrt{2\pi \tau_c}} e^{-i\Phi'_o(x)}
$$

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\[ \Phi_a = \frac{1}{\sqrt{2}} (\Phi'_e + \Phi'_o) \]
\[ \Phi_b = \frac{1}{\sqrt{2}} (\Phi'_e - \Phi'_o), \] (55)

U would take the form:
\[ U = \frac{V_1}{\sqrt{2\pi}} \frac{\partial \Phi_a(0)}{\partial x} + \frac{V_2}{\sqrt{2\pi}} \frac{\partial \Phi_b(0)}{\partial x} + \frac{V_3}{\pi \tau_c} \sigma_z \cos[\sqrt{2}\Phi_b(0)] \] (56)

with gauge symmetry under \( \Phi_a \to \Phi_a + c \); interchange symmetry under \( \sigma_z \to -\sigma_z, \Phi_a \to \Phi_a + \frac{\pi}{\sqrt{2}}, \Phi_b \to \Phi_b - \frac{\pi}{\sqrt{2}} \); and time reversal symmetry under \( x \to -x, \Phi_{a,b} \to -\Phi_{a,b} \). By then performing a unitary transformation using
\[ \Lambda' = \exp \left[ i \frac{V_1}{\sqrt{2\pi}} \Phi_a(0) + i \frac{V_2}{\sqrt{2\pi}} \Phi_b(0) \right] \] (57)

the first two terms in Eq(56) vanish so that the transformed Hamiltonian becomes
\[ \Lambda' H \Lambda'^{-1} = H_o + \frac{V_3}{\pi \tau_c} \sigma_z \cos[\sqrt{2}\Phi_b(0)] + \Delta_o \sigma_x. \] (58)

Noting that the second term is nothing but the third term in Eq(53), one might be tempted to conclude that the dynamics of the impurity is independent of \( V_2 \). However, a term of the form \( \sigma_x \frac{\partial \Phi_b(0)}{\partial x} \) will appear in Eq(56) from a perturbation expansion in \( \Delta_o \) and \( V_2 \) which cannot be eliminated by the canonical transformation and is not irrelevant. Indeed, this term breaks the apparent symmetry of Eq(58) under \( \Phi_b \to -\Phi_b \) which corresponds to \( \Phi'_e \leftrightarrow \Phi'_o \) and is not an exact symmetry in the presence of \( V_2 \) or similar terms. In the Appendix B we consider a more general formulation of the two site problem which shows how, even if the part of the Hamiltonian that is symmetric under \( \sigma_z \to -\sigma_z \) is diagonalized fully before bosonizing, the energy dependence of scattering processes will, nevertheless, generally lead to terms which play a similar role to \( V_2 \).

We now analyze the effects of the even-odd symmetry breaking terms, such as \( V_2 \), and other terms that are generated from these, by use of a Coulomb gas representation. As we shall see, in certain regimes, extra relevant operators are generated from the marginal operators that will delocalize the heavy particle.
III. COMPUTATIONS

A. Path Integral Representation

In this section, we analyze the bosonized Hamiltonian Eq(53) by a Coulomb gas representation and show how extra operators are generated which physically correspond to the impurity hopping together with one or more electrons. These will delocalize the impurity in regimes in which it was previously believed to be localized. (They will also generate extra important operators in Hamiltonians with “electron assisted tunnelling” like that analyzed by Vladár and Zawadowski.) The Hamiltonian Eq(53) is in a convenient form since it includes, in a simple way, a term that breaks the artificial symmetry in the absence of \( V_2 \), as well as a simple form of the impurity coupling to the Fermi sea. To treat Eq(53) we first perform a canonical transformation from \( H \) to \( H' \) using the unitary operator

\[
\Lambda = \exp \left[ -i \left( \frac{V_1}{\sqrt{2\pi}} \Phi_x(0) + \frac{V_3}{\sqrt{2\pi}} \sigma_z \Phi_o(0) \right) \right].
\]

Then \( H \) becomes

\[
H' = \Lambda H \Lambda^{-1} = H_o + \frac{V_2}{\pi \tau_c} \cos[\sqrt{2\pi} \Phi_o(0)] + \Delta_o \left\{ \sigma_+ \exp \left[ i\sqrt{2\pi} Q_o \Phi_o(0) \right] + h.c. \right\}
\]

where \( \sigma_\pm = \frac{1}{2} (\sigma_x \pm i\sigma_y) \) and \( Q_o = -\frac{V_3}{\pi} \) which as will be seen later is the effective charge for the hopping process. In Appendix A it will become clear why \( Q_o \) really is the charge transferred when the impurity hops between far away sites, by expressing \( Q_o \) in terms of the scattering phase shifts.

The Hamiltonian Eq(60) is expressed entirely in terms of exponentials of boson operators which are particularly convenient for deriving a Coulomb gas representation. Note also that the even parts of the Bose field are completely decoupled from the odd parts and the impurity. Although the formally irrelevant operators in Eq(53) have been ignored, their effects under the canonical transformation would only be to modify the coefficient of the \( V_2 \) term, and to give operators that are still irrelevant and break no symmetries, although they would include coupling to the even part of the Bose field. We can however safely ignore these.
The correlations of the impurity position $\sigma_z$, will not be affected by the canonical transformation as $\sigma_z$ commutes with $\Lambda$. We therefore work with Eq(60) and drop the prime on $H$. Including the effects of spin $\sigma$, we have, dropping the “o” (odd) subscript on $\Phi$

$$
H = H_o + \frac{V_2}{\pi \tau_c} \sum_\sigma \cos[\sqrt{2}\Phi^\sigma(0)] + \Delta_o \left\{ \sigma_+ \prod_\sigma \exp \left[ i\sqrt{2}Q_o \Phi^\sigma(0) \right] + \text{h.c.} \right\}
$$

(61)

with

$$
H_o = \sum_\sigma \int_0^\infty \frac{d\epsilon}{2\pi} \phi^{\sigma^+}(\epsilon)\phi^{\sigma}(\epsilon)e^{-\epsilon\tau_c}
$$

(62)

and

$$
\Phi^\sigma(x) = \int_0^\infty \frac{d\epsilon}{\sqrt{2\pi\epsilon}} \left[ \phi^{\sigma}(\epsilon)e^{i\epsilon x} + \phi^{\sigma^+}(\epsilon)e^{-i\epsilon x} \right] e^{-\frac{\epsilon x^2}{2}}.
$$

(63)

We are interested in the zero temperature partition function $Z = Tr \left[ e^{-\beta H} \right]$ in the limit $\beta \to \infty$. If we expand $Z$ in $V_2$ and $\Delta_o$ we obtain a sum over one dimensional “paths” from $\tau = 0$ to $\beta$. Each of these paths corresponds to a process in which the impurity hops between the sites at particular times shifting the phase of electron excitations, while at other times the electrons hop via the $V_2$ term. Such a path is illustrated in Figure 2. For simplicity, we first work with a single spin species. Then we can write $Z$ as

$$
Z = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \prod_{k=1}^{2m} \left( \sum_{\zeta_k = \pm 1} \right) \Delta_o^{2n} y^{2m} \delta_0^{\sum_{k=1}^{2m} \zeta_k} \int_0^\beta ds_1 \ldots \int_0^{s_{2m-1}} ds_{2m} \int_0^\beta d\tau_1 \ldots \int_0^{\tau_{2n-1}} d\tau_{2n} Z_{nm} \left( \{\zeta_k\}, \{s_i\}, \{\tau_j\} \right)
$$

(64)

with

$$
Z_{nm} \left( \{\zeta_k\}, \{s_i\}, \{\tau_j\} \right) = \langle 0 \left| Tr \left[ e^{i\zeta_{2n} \sqrt{2}\Phi(s_{2m})} \ldots e^{i\zeta_1 \sqrt{2}\Phi(s_1)} e^{-iQ_o \sqrt{2}\Phi(\tau_{2n})} \ldots e^{iQ_o \sqrt{2}\Phi(\tau_1)} \right] \right| 0 \rangle.
$$

(65)

where the product over different $\zeta_k = \pm 1$ corresponds to the two different terms in

$$
\cos \left( \sqrt{2}\Phi \right) = \frac{1}{2} \left( e^{i\sqrt{2}\Phi} + e^{-i\sqrt{2}\Phi} \right)
$$

and the “fugacity” $y$ of the electron hops is defined as

$$
y \equiv \frac{V_2}{2\pi \tau_c}
$$

(66)
We have taken the impurity to be on the “one” site at \( \tau = 0 \), this merely reduces \( Z \) by a multiplicative factor of two. Note that the signs of the \( \pm i \sqrt{2Q_0} \Phi(\tau_n) \) must alternate corresponding to the particle hopping back and forth, i.e. alternating \( \sigma_+ \) and \( \sigma_- \) terms from Eq(\ref{eq:61}), and the sum is constrained to an even number of hops because the impurity begins and ends at the same site. In addition, we shall see that only terms with an even number of \( y \) “charges” will contribute, thus the sum \( \sum_{k=1}^{2m} \zeta_k \) has to vanish. We have suppressed the dependence of \( \Phi(x=0) \) on the variable \( x \) and by \( \Phi(\tau) \) we denote:

\[
\Phi(\tau) = e^{+H_o \tau} \Phi e^{-H_o \tau}
\]

(67)

with the expectation in Eq(\ref{eq:63}) taken with the ground state of \( H_o \). The evaluation of the expectation value of the time ordered product in Eq(\ref{eq:63}) is particularly simple due to the bosonic character of \( \Phi \). First we observe that Eq(\ref{eq:67}) becomes

\[
\Phi(\tau) = \int_0^\infty \frac{d\epsilon}{\sqrt{2\pi\epsilon}} \left[ \phi(\epsilon)e^{-\epsilon \tau} + \phi^+(\epsilon)e^{\epsilon \tau} \right] e^{-\epsilon \tau c}.
\]

(68)

Thus it is of the form \( \Phi(\tau) = B(\tau) + B^+(-\tau) \) where \( B(\tau) \) is a boson having commutation relations:

\[
[B(\tau), B(\tau')] = 0 \\
\text{and } [B(\tau), B^+(-\tau')] = \int_0^\infty \frac{d\epsilon}{\epsilon} e^{-\epsilon \tau c} e^{-\epsilon(\tau-\tau')} = I(\tau - \tau')
\]

(69)

for \( \tau > \tau' \), \( I(\tau - \tau') \) being formally divergent at small energies; but only the finite part

\[
\tilde{I}(\tau) \equiv I(\tau) - I(0) = \ln \left( \frac{\tau_c}{\tau + \tau_c} \right)
\]

(70)

will enter physical quantities. By the standard procedure of reordering the operators to bring \( B \) to the right and \( B^+ \) to the left using the commutators in Eq(\ref{eq:69}), and noting that for zero temperature, only the ground state of \( H_o \) will appear on the right and left, we see that terms with the total charge \( \sum_k \zeta_k \neq 0 \) will give negative infinite terms in the exponentials and thus zero contribution to \( Z \). Furthermore the partition function \( Z_{nm} \) can be written in terms of effective interaction between the charges with strength
\[ W_{ij} = 2q_i q_j \tilde{I} (|r_i - r_j|) \]  
(71)

where \( r_i = \tau_i \) with \( q_i = +Q_o \) for the \( \sigma_+ \) impurity hops \( 1 \to 2 \); \( r_i = \tau_i \) with \( q_i = -Q_o \) for the \( \sigma_- \) impurity hops \( 2 \to 1 \); and \( \tau_i = s_i \) with \( q_i = \zeta_i \) for the electron hops, \( y \). The partition function \( Z_{nm} \) is thus simply the Boltzmann factor for the charges interacting with the logarithmic potential Eq(71), i.e.

\[ Z_{nm} (\{\zeta_k\}, \{s_i\}, \{\tau_j\}) = e^{-\mathcal{E}_{nm}} \]  
(72)

with

\[ \mathcal{E}_{nm} = -2Q_o^2 \sum_{(l,l')}^{2n} (-1)^{l+l'} \ln \left( \frac{||\tau_l - \tau_{l'}| + \tau_c}{\tau_c} \right) \]

\[ -2 \sum_{(k,k')}^{2m} \zeta_k \zeta_{k'} \ln \left( \frac{|s_k - s_{k'}| + \tau_c}{\tau_c} \right) \]

\[ +2Q_o \sum_{k=1}^{2m} \sum_{l=1}^{2n} (-1)^l \zeta_k \ln \left( \frac{|s_k - \tau_l| + \tau_c}{\tau_c} \right) \]  
(73)

It is instructive to note that the exponential of minus the second term in Eq(73) has the same form as the amplitude \((A_m)^2\) in Eq(8) which is nothing else than the square of an \( m \) particle Greens function. The reason it is the square of \( A_m \) and not just \( A_m \) is that here we have the product of the Greens functions of two sets of particles, the \( c_1^+ \)'s and the \( c_2^+ \)'s.

The partition function \( Z \) in Eq(64) with \( Z_{nm} \) from Eq(73), is thus a 1-D Coulomb gas with logarithmic interactions between integer charges \( \pm \zeta_k \) with fugacity \( y \) and “hopping” charges with fugacity \( \Delta_o \) and charge \( \pm Q_o \) which must strictly alternate in sign.

To take into consideration the effects of more than one spin species, we must modify Eq(73) to include the effective interactions between the impurity hops \( \sigma_\pm \) from each spin and the \( \pm 1 \) charges from the \( V_2 \) term in \( H \) for each spin species. Since the Bose fields \( \Phi^\sigma \) are independent, the interactions will be simply additive. Thus we must replace the “charges” \( q_i \) in Eq(73) by vector charges \( \vec{q}_i \) with two components for spin-1/2 electrons. For the impurity hops we have

\[ \vec{q} = \vec{Q}_o \equiv (Q_o, Q_o) \]

or \( \vec{q} = -\vec{Q}_o \equiv (-Q_o, -Q_o) \)
for $1 \rightarrow 2$ or $2 \rightarrow 1$ respectively, while for the electron hops, we have

\[ \vec{q} = (\zeta, 0) \]

or

\[ \vec{q} = (0, \zeta) \]

for spin $\uparrow$ or $\downarrow$ electrons respectively with $\zeta = \pm 1$, depending on the direction of the electron hop. The total effective action now has the form

\[
S_{nm} = \mathcal{E}_{nm} - 2m \ln y - 2n \ln \Delta_o \\
= -2 \sum_{j > i} \vec{q}_i \cdot \vec{q}_j \ln \left( \frac{r_j - r_i + \tau_c}{\tau_c} \right) - 2m \ln y - 2n \ln \Delta_o
\]  

(74)

with the ordered times $r_i = s_i$ or $\tau_i$ and the $2n$ charges $\vec{q}_i = \pm \vec{Q}_o$ with fugacity $\Delta_o$, strictly alternating in sign. The $2m$ charges in Eq(74) with fugacity $y$, need not alternate in sign but the sum of all their charges must be zero.

**B. Renormalization Group Analysis**

We are now in the position to analyze the behavior of the impurity in terms of the properties of the generalized Coulomb gas with the action of Eq(74). We are particularly interested here in whether or not the impurity can be localized. Thus we consider the effects of a small hopping rate $\Delta_o$ and analyze the Coulomb gas perturbatively in both $\Delta_o$ and $y$. Standard balancing of the energy and “entropy” terms indicate that $y$ is exactly marginal — as it must be —, while the hopping $\Delta_o$ has renormalization group (RG) eigenvalue

\[
\lambda_o = 1 - 2Q_o^2
\]  

(75)

under rescaling of the small time cutoff, $\tau_c$, with the factor of 2 coming from the two spin species. Since for $Q_o > 1/\sqrt{2}$, $\lambda_o < 0$, it would appear that the impurity hopping is irrelevant in this case, thereby leading to the conventional conclusion that a charge two impurity, which has $\vec{Q}_o = (1, 1)$ corresponding to the two spin channels, can be localized. As we shall see, however, extra charges will be generated under renormalization which invalidate this conclusion.
Since there are two types of charges $\vec{\zeta}$ and $\pm \vec{Q}_o$, of which only the $\pm \vec{Q}_o$ are restricted to alternate in sign, there are various processes which can be regarded as composite charges. For example, a charge $\vec{q} = (Q_o - 1, Q_o)$ can be formed if an impurity hop and an electronic hole hop are close to each other. This process as well as the more general processes which generate charges $(Q_o \pm n, Q_o \pm n)$ with $n = 1, 2, 3, \ldots$ were discussed physically in the Introduction. It is clear that while they do not exist in the original Hamiltonian they are generated under renormalization (or from perturbation theory). For example the hopping matrix element $\Delta_{(-1,0)}$ of a process with charge $(Q_o - 1, Q_o)$ will be generated under renormalization with magnitude proportional to $y \Delta_o$. Thus, in general, we must consider all possible composite charges and their effects on each other.

We denote charges associated with general types of impurity hops: $\vec{Q}$ and $-\vec{Q}$ for $\sigma_+$ and $\sigma_-$ hops, respectively, which occur at times $\tau_i$; $\vec{\zeta}$ for purely electronic hops at times $s_i$; and charge $\vec{q}$ for generic hops of either type at times $r_i$ with fugacity $z$. We need to analyze the effects of integrating out all pairs of charges with spacings between $\tau_c$, the cutoff and hence the minimum allowed spacing, and $\tau_c (1 + \delta l)$ with $e^l$ the time rescaling factor. Pairs of charges, $\vec{q}_1$ and $\vec{q}_2$, which do not sum to charge zero, will generate composite charges $\vec{q}_1 + \vec{q}_2$ with fugacity $z_1 z_2 k_{12} \tau_c \delta l$ with the $k \tau_c \delta l$ factor from the possible separations and ordering of $\vec{q}_1$ and $\vec{q}_2$, with $k = 2$ unless both $\vec{q}$’s are impurity hops, in which case $k = 0$ if they are both $\sigma_+$ and $k = 1$ (since only one ordering is possible), if one is $\sigma_+$ and the other $\sigma_-$. Neutral pairs, i.e. those with total charge zero, will not produce composite charges but will screen the interactions between the remaining charges.

We can proceed as usual by considering the effects of one neutral pair on other charges, specifically on a charge $\vec{q}$ at time $r$. If the pair is $\pm \vec{\zeta}$, i.e. purely electronic, then the effect of the two possible orderings cancel (up to modifying sub-logarithmic corrections to the interaction between remaining charges) and we thus ignore these. The interesting case is thus a pair of hops. The allowed orderings of a $\pm \vec{Q}$ pair at times $\tau \pm \tau_c/2$ with fugacities $\Delta_{\vec{q}} = \Delta_{-\vec{q}}$, depends on $\sigma_z(\tau)$. Thus the interaction of this pair with charge $\vec{q}$ at time $r$ is
\[
\delta I_{\vec{q}}(r) = -2\tau_c \vec{Q} \cdot \frac{\vec{q} \sigma_z(\tau)}{\tau - r}
\]  

(76)

for \(|\tau - r| \gg \tau_c\), the appropriate limit for analyzing the renormalization of the long time interactions. Expanding \(e^{-S}\) in \(\delta I_{\vec{q}}(r)\) and integrating over the possible position, \(\tau\), of the pair and the intra-pair spacing in the range \(\tau_c\) to \(\tau_c(1 + \delta l)\) we see that there are contributions every time \(\sigma_z(\tau)\) changes sign, i.e. at times \(\tau_i\). This generates an effective interaction between \(\vec{q}\) and all impurity hops, but not between \(\vec{q}\) and purely electronic hops. For an impurity hop \(\pm \vec{Q}_i\) at time \(\tau_i\), the generated effective interaction is

\[
\delta I_{\vec{q},\pm \vec{Q}_i} = \pm 4\tau_c^2 \Delta_{\vec{Q}}^2 \vec{Q}_i \cdot \vec{q} \ln |\tau_i - r| \delta l.
\]  

(77)

This thus has the effect of modifying the interaction of each \(\vec{Q}_i\) with all other charges by a way that is equivalent to changing \(\vec{Q}_i\) by

\[
\delta \vec{Q}_i = -2\tau_c^2 \Delta_{\vec{Q}}^2 \vec{Q}_i \delta l.
\]  

(78)

with \(\pm \vec{Q}\) the charges of the electron impurity impurity hop pair that have been integrated out. Since each \(\vec{Q}_i\) is of the form \(\vec{Q}_o\) plus an integer vector, we see that the net effect is just to change \(Q_o\) by

\[
\delta \vec{Q}_o = -2\tau_c^2 \delta l \sum_{\vec{N}} (\vec{Q}_o + \vec{N}) \Delta_{\vec{N}}^2
\]  

(79)

with the sum running over all possible types \(\vec{Q}\) of \(\sigma_+\) charges, i.e. \(\vec{Q} = \vec{Q}_o + \vec{N}\) with \(\vec{N}\) an integer vector; here and henceforth we use the abbreviated notation

\[
\Delta_{\vec{N}} \equiv \Delta_{\vec{Q}_o + \vec{N}}.
\]  

(80)

To this order in \(\Delta_{\vec{N}}\) and \(y_{\vec{N}}\), the fugacities for multi-electron hops which can have all integer vectors \(\vec{N}\) except \((0, 0)\), the RG flow equations are, after absorbing \(\tau_c\)'s into \(\Delta\) and \(y\) to make them dimensionless
\[
\frac{d\vec{Q}_o}{dl} = -2 \sum_N (\vec{Q}_o + \vec{N}) \Delta_N^2
\]
\[
\frac{d\Delta_{\vec{N}}}{dl} = \left( 1 - |\vec{Q}_o + \vec{N}|^2 \right) \Delta_{\vec{N}} + 2 \sum_{\vec{N}'\neq\vec{0}} y_{\vec{N}'} \Delta_{\vec{N}' - \vec{N}'}
\]
\[
\frac{dy_{\vec{N}}}{dl} = \left( 1 - |\vec{N}|^2 \right) y_{\vec{N}} + \sum_{\vec{N}'\neq\vec{0}} y_{\vec{N}'} y_{\vec{N}' - \vec{N}'} + \sum_{\vec{N}'} \Delta_{\vec{N}'} \Delta_{\vec{N}' - \vec{N}'}
\]
(81)

with

\[
\Delta_{\vec{N}} \equiv \Delta_{\vec{Q}_o + \vec{N}} = \Delta_{-(\vec{Q}_o + \vec{N})}
\]
(82)

by the 1 ↔ 2 interchange symmetry. As can be seen from Eq(81) all the multi-electron hop terms are irrelevant, thus we need only retain \( y_{(10)} = y_{(01)} \equiv y \); from Eq(81) we see that this is sufficient to generate all the composite charges with fugacities of order \( \Delta_o \) times powers of \( y \).

From Eq(81) we see that, generically for two spin channels, there are at least three relevant operators for any \( Q_o \): \( \Delta_{([Q_o] - 1, [Q_o])} \) and \( \Delta_{([Q_o], [Q_o] - 1)} \) with \([Q_o]\) the fractional part of \( Q_o \) are always relevant while either \( \Delta_{([Q_o], [Q_o])} \) or \( \Delta_{([Q_o] - 1, [Q_o] - 1)} \) or both will also be relevant. More generally, we arrive at the same conclusion as from the simple physical argument of the Introduction: in order to localize the impurity, more than four channels (including spin) are needed so that, if each channel, \( \gamma \), is optimally coupled by a \( \frac{1}{2} \)-integer \( Q_\gamma \), then \( \sum Q_\gamma^2 > 1 \) and the impurity can be localized.

The RG equations (Eq(81)) are quite different from those in the literature: if there were no \( V_2 \) term, then the extra composite impurity hopping terms would not be generated, and the impurity could appear to be localized by just s-wave scattering. Note that the apparent \( c_1 \to e^{i\phi}c_1 \) symmetry when \( V_2 = 0 \) actually allows for charges \( \vec{Q} = \vec{Q}_o + \vec{N} \) with even integer vector \( \vec{N} \), but these will not prevent localization. This point suggests that \( Q_o \) should be defined up to an even integer (i.e. mod 2). In fact it will be seen in Appendix A that \( Q_o \) is actually \( \pi^{-1} \) times a phase shift which naturally leads to its consideration of mod 2.

In the Hamiltonian considered by Vladár and Zawadowski [8] single electron assisted hopping terms that correspond to \( \Delta_{(-1,0)} \) and \( \Delta_{(0,-1)} \) are present but their Hamiltonian has the
implicit symmetry $c_1 \rightarrow -c_1, d_1 \rightarrow -d_1$. Then only a subset of the $\Delta_{\vec{N}}$ can be generated, specifically those with $N_\uparrow + N_\downarrow$ odd; again this artificial extra symmetry will change the behavior by limiting the number of possibly relevant operators.

**IV. DISCUSSION AND CONCLUSIONS**

In the previous section, we have seen that an impurity hopping between two symmetrically placed sites cannot be localized unless it is coupled strongly to more than four spin and angular momentum “channels”. If the sites are nearby — as they must be if the bare hopping rate is to be appreciable — then one cannot use angular momentum channels, and must, instead, generalize the treatment. One way to do this, which shows directly the role of the irrelevant operators and relies on no symmetries other than the site interchange symmetry, is to use the one-electron eigenstates of the symmetrized electron Hamiltonian $H_S$ which is the average of the Hamiltonians with the impurity on the two sites. The antisymmetric part then scatters the electrons between even and odd parity states of $H_S$. The analysis in this representation is carried out in Appendix B, with the same conclusions being reached as in Section III.

The problems with most earlier treatments of the two-site system have been of two types: In many of the treatments, an extra $U(1)$ symmetry associated with the independence of the electrons which interact with the impurity at the two sites is implicitly assumed. The $V_2$ term that breaks this symmetry is marginal but it creates extra operators, particularly those which move one localized hole with the impurity, and these processes delocalize a charge two particle which had previously claimed to be localized if it interacts with only $s$-wave electrons at each impurity.

Recently, there has also been a substantial literature on the relationship between an impurity with “electron assisted tunnelling” — i.e. hopping of the impurity concomitantly with the motion of one electron of either spin — and the two channel Kondo problem with the $z$-component of the Kondo “spin” being the impurity position and its $x$-component
the hopping, (i.e. our \( \sigma_z \) and \( \sigma_x \)). The two “channels” of the Kondo problem are then the two electron spin species which are exactly degenerate in the absence of an external field. The frequently used Hamiltonian for this problem was introduced by Vladár and Zawadowski. However, they completely neglected a \( V_2 \)-like term. They derive the electron-assisted hopping term assuming that \( Q_o \ll 1 \) and \( k_F R \ll 1 \). Even in this case, using their numbers we find that the estimate of the amplitude of the electron-assisted hopping term they get is smaller by at least one to two orders of magnitude from the amplitude of \( \Delta_{(-1,0)} \) that is generated from Eq(81) after renormalizing to \( l = O(1) \):

\[
\Delta_{(-1,0)} \sim y \Delta_o \sim \Delta_o \pi \rho_F V
\]  

with \( k_F R \leq 1 \). In the case of \( k_F R \geq 1 \), essential to get \( Q_o = O(1) \) which is the relevant situation for localization, their derivation of the electron-assisted hopping term breaks down. In our treatment and because of the existence of \( V_2 \) we show how both \( \Delta_{(-1,0)} \) and other relevant terms (e.g. \( \Delta_{(-1,-1)} \)) naturally arise. Thus, in any case, we believe we have here a more complete physical picture of the problem.

As we have seen, these extra terms change the physics for large \( Q_o \) and small hopping — the “weak coupling” (small \( J \)) limit in the Kondo language. Most of the recent literature has focused on the “strong coupling” behavior of the Kondo system i.e. the regime at low energies with parameters, particularly \( Q_o \), such that exchange is relevant and flows to large values corresponding to the particle hopping back and forth between the two sites. Novel non-Fermi liquid behavior has been found theoretically in this regime for which our considerations are not directly relevant. Nevertheless, the extra symmetry implicit in these treatments is potentially dangerous, indeed, as we will show elsewhere, terms that break this symmetry change the physics in the strong coupling delocalized regime, as they did in the weak hopping regime analyzed in this paper.

One of the major motivations for the present work was the hope of gaining further understanding about the properties of a heavy particle that can hop on sites of a periodic lattice impeded (or in some regimes assisted!) by the coupling to a Fermi sea. This has
potential relevance for the mobility of muons in metals, the sharpness (or rounding) of X-ray edge singularities when the deep hole can move (albeit with a large bare mass), and possibly the properties of a heavy d- or f-electron band coupled to a light conduction band.

The main papers (e.g. reference 1 and references therein) on the behavior of a single particle in such a periodic system, suffer from some of the same problems as those on the two-site system: they treat a subset of the allowed operators and do not allow for the effects of others that may be generated. Not surprisingly, the conclusions of these papers are the same as for the two site case: that a charge two particle with only s-wave scattering can be localized while a charge one particle cannot be. In light of the present results, this conclusion should clearly be reexamined.

In the spirit of the work of Sols and Guinea, one could treat each step of the particle motion — whether via nearest or further neighbor hopping — essentially independently and look at the renormalization of each such hopping term separately, including the possible motion of electrons with the particle, by the methods outlined in this paper. From this approach the following conclusion would be immediate: that the particle cannot be localized unless all the hopping processes are irrelevant, and this can only occur if there are more than four electron channels involved for every possible hopping process and the coupling is sufficiently strong. Thus with just s-wave scattering, a particle cannot be localized, in contrast to the conclusion in the literature. Instead, the particle will move around with a screening cloud of electrons in tow.

Unfortunately, there are problems in extending the two site results in this way. The primary one is the spatial structure of the system and the lack of independence between the electrons involved in hopping between different pairs of sites. For any finite number of sites, the electrons can be treated as essentially one dimensional at sufficiently low energies, and generalization of the present methods can be used to categorize all the operators. We have explicitly carried out this procedure for a simple case of three sites symmetrically arranged in a triangle and find that the same conclusions are obtained as in the two site case. We believe that this should likewise hold for any finite number of sites. However for an infinite
lattice of sites, the electrons must be considered to be fully three dimensional and the limit
of small bare hopping rate that we have studied perturbatively, may not be exchangeable
with the limit of an infinite number of sites. In particular, one has to worry about at least
two effects. First, even if the particle is moving very slowly, there will always be particle-hole
excitations with group velocities slower than the particle; these can perhaps not be treated
in the same manner as the rapidly moving excitations. Second, one could argue that there
are an infinite number of scattering “channels” involved because of electrons near each of the
sites. Perhaps these might make it easier to localize the particle, although it is not clear how
this could come about. Conversely, they might somehow interfere and prevent localization
even if there are many scattering channels at each site. We must, unfortunately, leave these
questions for future study. But we should note, that if the preliminary conclusion about
the difficulty of localizing a heavy particle is correct, it may have implications for some of
the suggested possibilities for interesting new physics with a heavy f-electron band coupled
to a light conduction electron band\textsuperscript{20}. Again, we leave this, as well as the possibility of
interesting effects on the electrons caused by a delocalized impurity, for future work.

The present analysis, although not introducing new techniques, has, we hope, made the
physical picture behind the competition between orthogonality catastrophe and hopping
clearer and simpler. In addition, the pitfalls of the standard combination of bosonization
techniques and “large” canonical transformations have been brought out and should be
heeded by workers on other problems in this area.

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APPENDIX A:

In this Appendix it is illustrated how one can get a Coulomb gas representation of the partition function $Z$ directly from the original form of the Hamiltonian Eq(32), without bosonizing. At the same time the physical interpretation of $Q_o$ as the transferred electron screening charge instead of simply being the interacting potential $V_3$ — which is the naive result of bosonization — will become apparent. The method used here has been applied to systems very similar to ours in the past, so we will not go into the details of the calculations.

It is straightforward to see that using the Hamiltonian in Eq(32) one can get an expression for the partition function $Z$ similar to Eq(64):

\[ Z = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \Delta_{2n}^{2n} y^{2m} \int_0^\beta ds_1 \ldots \int_0^{s_{2m-1}} ds_2 m \int_0^\beta d\tau_1 \ldots \int_0^{\tau_{2n-1}} d\tau_2 n Z_{nm}(\{s_i\}, \{\tau_j\}) \]  

(A1)

where $y \propto V_2$ and

\[ Z_{nm}(\{s_i\}, \{\tau_j\}) = \left\langle 0 \left| T \left[ c_1^+(s_1) c_2(s_1) \ldots c_2^+(s_{2m}) c_1(s_{2m}) \right] \exp \left( -\int_0^\beta d\tau' H'_o(\tau') \right) \right| 0 \right\rangle. \]  

(A2)

In Eq(A2) by $H'_o$ we denote

\[ H'_o(\tau) = H_o + (V_1 + V_3) c_1^+ c_1 + (V_1 - V_3) c_2^+ c_2 + 2V_3 \theta(\tau) \left( c_2^+ c_2 - c_1^+ c_1 \right) \]  

(A3)

with

\[ \theta(\tau) = \begin{cases} 
0 & \text{for } \tau \epsilon (\tau_{2k}, \tau_{2k+1}) \quad k = 0, 1, \ldots, n \\
1 & \text{for } \tau \epsilon (\tau_{2k-1}, \tau_{2k}) \quad k = 1, \ldots, n
\end{cases} \]  

(A4)

Since the $V_2$ term contains both $c_2^+ c_1$ and $c_1^+ c_2$ which can be generated at any time $s_i$, there is no constraint in the order in which they appear in Eq(A2). However, due to the number-conserving character of $H'_o(\tau)$ there is a constraint of having, for each $i$, as many $c_i^+$ as $c_i$’s in the time ordered product of $Z_{nm}$. For convenience we pick $|0>$ to be the ground state of $H_o + (V_1 + V_3) c_1^+ c_1 + (V_1 - V_3) c_2^+ c_2$. We can see that $Z_{nm}$ represents a Green’s function of $m$ particles, types “1” and “2”, in a time dependent potential which changes its value when the
impurity hops at times $\tau_i$. This, in the language of the Kondo problem, is equivalent to a path in which the impurity spin flips at times $\tau_i$ while the electrons flip their “spin” (i.e. 1–2 index) at times $s_j$. The amplitude for such a process is a product of two independent parts, i.e. the amplitude of the 1-particles and that of the 2-particles. Now since the “interaction” term $V_3$ is really only a one particle operator, all the diagrams will be either closed loops or else will end at times $s_i$, so we can thus treat them independently. The closed loop contribution is simply $Z_{n0}$ which is identical to that of the Kondo problem.

In order to get the other contribution let us first consider $m=1$. Then the amplitude corresponds to a one-particle Green’s function in the presence of the time dependent Hamiltonian which can be shown to have the following long time (i.e. all time differences $|\tau - \tau'| \gg \tau_c$) solution:

$$G(s, s') \propto \frac{1}{s - s'} \prod_{k=1}^n \left| \frac{(\tau_{2k} - s) (\tau_{2k-1} - s')}{(\tau_{2k} - s') (\tau_{2k-1} - s)} \right|^\delta$$  \hspace{1cm} (A5)

with the phase shift

$$\delta = - \arctan \frac{V_2}{\beta} + \pi \Theta(-\beta)$$  \hspace{1cm} (A6)

with $\Theta$ the Heavyside step function and

$$\beta = 1 - V_1 \tan \theta + \frac{1}{4} \left( 1 + \tan^2 \theta \right) \left( V_1^2 - V_3^2 \right)$$  \hspace{1cm} (A7)

with $\theta$ related to the short time behavior of $G_o$ (the propagator of $H_o$) including the existence of bound states and particle-hole asymmetry. Note that the extra $\Theta$-function, which in the past had often been ignored and was only recently introduced explicitly makes $\delta$ defined between $-\frac{\pi}{2}$ and $\frac{\pi}{2}$.

From Eq(A6) it becomes clear that although $V_1$ may be formally decoupled from the impurity in the bosonized version of the problem (see Eq(53)) it does renormalize the exponent $\delta$. This leads us to the conclusion that indeed $\delta$ is a non-universal quantity — not in general simply related to the phase shifts for scattering off a static impurity.

More generally, since electron operators anti-commute, the amplitude for $m$ particles is a determinant of $G(s_i, s'_j)$ terms (see Eq(8)): $\det G \left( s_i, s'_j \right)$, where $s_i$ and $s'_j$ are times at
which the i-th 1-particle was created and the j-th 1-particle was annihilated, respectively. Expanding the determinant (over \(i,j\)) out, we get

\[
\det G(s_i, s'_j) = \prod_{i>j} (s_i - s_j) \prod_{i} \prod_{k=1}^{n} \left( \frac{\tau_{2k} - s_i}{\tau_{2k-1} - s_i} \right) \prod_{i>j} (s'_i - s'_j) \prod_{i} \prod_{k=1}^{n} \left( \frac{\tau_{2k} - s'_i}{\tau_{2k-1} - s'_i} \right) \prod_{i,j} (s_i - s'_j) \prod_{n} \prod_{k=1}^{n} \left| \tau_2^k - \frac{s_i}{\pi} \right|^{\frac{\delta}{\pi}} \quad \text{(A8)}
\]

We can now bring this in a form closer to Eq(73) if we introduce a number \(\zeta_i\) which is +1 for \(s_i\) and -1 for \(s'_i\). Then, quoting the result for the closed loop amplitude

\[
\exp \left[ \left( \frac{\delta}{\pi} \right)^2 \sum_{l > l'} (-1)^{l+l'} \ln |\tau_l - \tau_{l'}| \right], \quad \text{(A9)}
\]

and using Eq(A8), after taking the square of all the above amplitudes to take into account the two channels \((1,2)\), \(Z_{nm}\) becomes:

\[
Z_{nm} (\{\zeta_i\}, \{s_i\}, \{\tau_j\}) = \exp \left[ +2 \left( \frac{\delta}{\pi} \right)^2 \sum_{(l,l')} (\frac{\delta}{\pi})^{l+l'} \ln |\tau_l - \tau_{l'}| \right] \times \exp \left[ +2 \sum_{(k,k')} \zeta_k \zeta_{k'} \ln |s_k - s_{k'}| \right] \times \exp \left[ -2 \frac{\delta}{\pi} \sum_{k=1}^{2n} \sum_{l=1}^{2m} (-1)^{l} \zeta_k \ln |s_k - \tau_l| \right] \quad \text{(A10)}
\]

This is equivalent to Eq(73) if \(\frac{\delta}{\pi} \rightarrow Q_o\). The essential reason for the appearance of an arctangent of the potential in Eq(A6) is because the singular effects of higher order terms in \(V_3\) are included. Eq(A6) makes \(\delta\) finite even if \(V_3\) is infinite. Finally, from Friedel’s sum rule, it would seem that \(\frac{\delta}{\pi}\) corresponds to the electronic screening charge moved when the impurity hops from site to site, thus \(Q_o\) would be just this screening charge. One should emphasize, however that this correct only in the limit of large site separation for which \(V_2\) is small and \(\delta\) is not appreciably renormalized from the phase shift off a static impurity at one of the two sites.

In conclusion, we have seen here that \(|Q_o| \leq \frac{1}{2}\), since \(-\frac{n}{2} < \delta \leq \frac{n}{2}\). However this is essentially equivalent with the results of this paper in which we have shown that for any initial bare value of \(Q_o\) the most relevant process that will dominate in delocalising the impurity, is the one that has charge \(q\) with absolute value
\[ |q| = \min_{n \in \mathbb{Z}} \{|[Q_o]|, |[Q_o] - n|\} \leq \frac{1}{2} \tag{A11} \]

with \([Q_o]\) the fractional part of \(Q_o\) (see discussion after Eq(81)). The physical picture presented in this paper provides an intuitive way of understanding why the branch of \(\delta\) implied by Eq(A6) is dominant. This was not apparent in some of the earlier work\footnote{\ref{footnote}--\ref{footnote}} and is the source of some of the erroneous claims about particle localization\footnote{\ref{footnote}--\ref{footnote}}.

**APPENDIX B:**

In this Appendix, we show how the site problem can be analyzed generally in terms of “channels” even in the absence of any symmetry except the equivalence of the two sites. In addition, we will see how bosonization in a representation in which no \(V_2\)-like electron hopping term can exist will still, if handled carefully, yield terms which play the same role. Furthermore, the possibility of exchange of “charge” between various channels will be found, yielding another, albeit related way, that charges can be reduced, and localization impeded.

We consider the electronic Hamiltonians with the impurity at either site one or two, denoted \(H_1\) and \(H_2\), and diagonalize exactly the *symmetrized* Hamiltonian

\[ H_S = \frac{1}{2} (H_1 + H_2). \tag{B1} \]

The full Hamiltonian is then written as

\[ H = H_S + \sigma_z H_A + \Delta_o \sigma_x \tag{B2} \]

with the antisymmetric part

\[ H_A = \frac{1}{2} (H_1 - H_2). \tag{B3} \]

With fermion operators that diagonalize \(H_S\), we see that neither \(V_2\)- nor \(V_1\)-like terms can occur. At each energy, there will be a countable degenerate set of scattering eigenfunctions of \(H_S\), which we label by \(k = \epsilon - \epsilon_F\), setting \(v_F = 1\); and for the states that are even (e) under
interchange 1 ↔ 2 we use a “channel” index \( \eta \) which we can choose later for convenience, while we use an index \( \theta \) for the odd (o) states. Thus

\[
H_S = \sum_k \sum_{\eta} k c_{k\eta e}^+ c_{k\eta e} + \sum_k \sum_{\theta} k c_{k\theta o}^+ c_{k\theta o}
\]

and the antisymmetric part has the general form

\[
H_A = \sum_{k,k'} \Gamma_{\eta,\theta}(k,k') \left[ c_{k\eta e}^+ c_{k'\theta o} + h.c. \right] .
\]

Since we are interested in the behavior near the Fermi surface, we can choose linear combinations of the even states at \( k = 0 \) and likewise the \( k = 0 \) odd states, so that

\[
\Gamma_{\eta,\theta}(0,0) = \delta_{\eta\theta} \gamma_{\eta}
\]

is diagonal in \( \eta, \theta \); then in this representation we can denote \( \theta \) also by \( \eta \). We now form the operators

\[
\Psi_{\eta e} = \frac{1}{\sqrt{N_{e(o)}}} \sum_k c_{k\eta e(o)}
\]

with appropriate normalization factors \( N_{e(o)} \) as in Eq(23), and define

\[
\Psi_{\eta 1} = \frac{1}{\sqrt{2}} (\Psi_{\eta e} + \Psi_{\eta o})
\]

\[
\Psi_{\eta 2} = \frac{1}{\sqrt{2}} (\Psi_{\eta e} - \Psi_{\eta o}).
\]

The Hamiltonian then takes the form

\[
H = H_S + \sigma_z \sum_\eta \gamma_\eta \left( \Psi_{\eta 1}^+ \Psi_{\eta 1} - \Psi_{\eta 2}^+ \Psi_{\eta 2} \right) + \sigma_z M
\]

where the correction term \( M \) involves the deviations of \( \Gamma \) from the diagonal form for \( k, k' \neq 0 \):

\[
M = \sum_{k,k'} \sum_{\eta,\eta'} (\Gamma_{\eta\eta'}(k,k') - \gamma_\eta \delta_{\eta\eta'}) \left( c_{k\eta e}^+ c_{k'\eta' o} + h.c. \right) .
\]

If we bosonize the \( \Psi_{\eta 1,2} \) following the prescription used in Section II.B, then in the absence of \( M \), the Hamiltonian just takes the simple form

\[
H = \Delta_o \sigma_x + \sum_\eta H_\eta
\]
with
\[ H_\eta = K_\eta + \frac{\gamma_\eta}{\sqrt{2\pi}} \sigma_z \frac{\partial \Phi_{\eta o}(0)}{\partial x} \]  \hspace{1cm} (B12)

where \( K_\eta \) is the kinetic energy of the \( \eta \) bosons. We then have for each channel \( \eta \) an independent charge
\[ Q_{\eta o} = \frac{\gamma_{\eta o}}{\pi}, \]  \hspace{1cm} (B13)

so that\[ \alpha_o = \sum_\eta Q_{\eta o}^2. \]  \hspace{1cm} (B14)

In the absence of \( \mathcal{M} \), the particle would thus be localized if \( \alpha_o > 1 \).

Analysis of the form of \( \mathcal{M} \), shows, with the \( \eta \) basis chosen to vary slowly with \( k \), the existence of formally irrelevant terms like
\[ \sigma_z \frac{\partial \Phi_{\eta o}(0)}{\partial x} \cos \left[ \sqrt{2} \Phi_{\eta o}(0) \right], \]  \hspace{1cm} (B15)

the \( \frac{\partial}{\partial x} \) essentially arising from terms in \( \mathcal{M} \) linear in \( k \) and \( k' \). Under the canonical transformation that eliminates the \( \sigma_z \frac{\partial \Phi_{\eta o}(0)}{\partial x} \) terms in Eq (B12), these will generate \( \cos \left[ \sqrt{2} \Phi_{\eta o}(0) \right] \) terms which are of exactly the same form as these that would have arisen from a \( V_2 \) term originally. These terms create integer charges which can then combine with the \( Q_\eta \) charges to give effective charges of \( Q_\eta - n_\eta \) with integer \( n_\eta \). Because of the choice of the \( \eta \) fermions, these terms no longer have quite the interpretation of moving \( n_\eta \) electrons with the impurity. Physically, this is quite simple: in the correct basis, the electrons do not need to be moved, they will do so on their own due to the change in the electronic part of \( H \) as the impurity moves.

In addition to \( V_2 \)-like terms, terms of the form
\[ e^{i \frac{\pi}{\sqrt{2}} (\Phi_{\eta \epsilon} - \Phi_{\eta' \epsilon})} \sin \left( \frac{\Phi_{\eta o}}{\sqrt{2}} \right) \sin \left( \frac{\Phi_{\eta' o}}{\sqrt{2}} \right) \]  \hspace{1cm} (B16)

will also be generated under the canonical transformation from \( \Gamma_{\eta \eta'} \) terms linear in \( k \). These will create \( \frac{1}{2} \) charges in the formerly-decoupled even channels. For any pair \( \eta, \eta' \), it can be
seen that the effective charge squared of combining this process with a hop has a contribution to $\alpha_o$ from these two pairs of even and odd channels of
\[
(Q_\eta - \frac{1}{2})^2 + \frac{1}{4} + (Q_\eta' - \frac{1}{2})^2 + \frac{1}{4}.
\]
(B17)
Since the resulting contribution from each even-channel charge is $\frac{1}{4}$, it can be seen that the effective charge squared of each channel cannot, in the general case, be reduced below $\frac{1}{4}$, i.e. the same result as in the absence of the channel mixing terms. Therefore these terms do not change the conclusion of the earlier discussion. Nevertheless, the presence of channel mixing terms will complicate the analysis of the many site problem and could perhaps change the physics in a spatially extended system.
REFERENCES

1 F. Sols and F. Guinea, Phys. Rev. B 36, 7775 (1987).

2 K. Yamada, A. Sakurai and M. Takeshige, Prog. Theor. Phys. 70, 73 (1983).

3 P. W. Anderson, Phys. Rev. Lett. 18, 1049 (1967).

4 D. R. Hamann, Phys. Rev. Lett. 26, 1030 (1971).

5 A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg and W. Zwerger, Rev. Mod. Phys. 59, 1 (1987).

6 K. Vladár and A. Zawadowski, Phys. Rev. B 28, 1564 (1983); B 28, 1582 (1983); B 28, 1596 (1983).

7 L. D. Chang and S. Chakravarty, Phys. Rev. B 31, 154 (1985).

8 K. D. Schotte and U. Schotte, Phys. Rev. 182, 479 (1969); 185, 509 (1969).

9 Yu. Kagan, J. Low Temp. Phys. 87, 525 (1992).

10 A. Murumatsu and F. Guinea, Phys. Rev. Lett. 57, 2337 (1986).

11 V. L. Líbero and L. N. Oliveira, Phys. Rev. Lett. 65, 2042 (1990).

12 I. Affleck and A.W.W. Ludwig, Phys. Rev. Lett. 68, 1046 (1992).

13 $\alpha, \beta, \theta$ must satisfy $\alpha^2 + \beta^2 = \frac{\pi}{k^2} \left[1 - \left(\frac{\sin kR}{kR}\right)^2\right]^{-1}$ and

$$2\alpha \beta \cos \theta = -\frac{\pi}{k^2} \frac{\sin kR}{kR} \left[1 - \left(\frac{\sin kR}{kR}\right)^2\right]^{-1}.$$

14 P. Noziéres and C. T. De Dominicis, Phys. Rev. 178, 1097 (1969).

15 R. Shankar: Bosonization: How to make it work for you in condensed matter. Lectures given at the BCSPIN school, Katmandu, May 1991.

16 V. J. Emery and S. Kivelson, Phys. Rev. B 46, 10812 (1992).

17 A. W. W. Ludwig and I. Affleck, Phys. Rev. Lett. 67, 3160 (1991); I. Affleck and A. W.
W. Ludwig, Phys. Rev. B 48, 7297 (1993).

18 D. L. Cox, Phys. Rev. Lett. 59, 1240 (1987).

19 N. Andrei and C. Destri, Phys Rev. Lett. 52, 364 (1984); P. B. Wiegmann and A. M. Tsvelick, Z. Phys. B 54, 201 (1985).

20 Q. Si and G. Kotliar, Phys. Rev. Lett. 70, 3143 (1993).

21 G. Yuval and P. W. Anderson, Phys. Rev. B 1, 1522 (1969).

22 I. Perakis and Y.C. Chang, Phys. Rev. B 47, 6573 (1993).

23 Note that $\alpha_o$ defined in Eq(9) had an extra factor of 1/2 multiplying the sum. The reason this should not appear here is that there we were essentially overcounting, by a factor of two, the number of channels by treating the 1- and 2-electrons separately. It is clear that this factor of two should not appear in Eq(B14) as $Q_{\eta o}$ is defined as the charge transfer of the combined process of both 1- and 2-electrons.