Renormalization group techniques applied to the Anderson model of magnetic alloys.

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This paper addresses the problem of spin-½ magnetic impurities in a nonmagnetic metal as given by the Anderson model and how it may be approached using the techniques of the renormalization group. After a brief introduction to the basic concepts of the renormalization group, the Anderson problem is described and manipulated into a form that is suitable to renormalization group analysis. An iterative solution for the Anderson Hamiltonian and its physical properties is then outlined, followed by a presentation of numerical results.

I. Introduction to the Renormalization Group

The techniques of the renormalization group enable us to study the statistical continuum limit, which is a phenomenon that arises in many forms in a variety of problems in physics. Although its manifestations are varied, the most important feature of the statistical continuum limit is the absence of characteristic energy or length scales. For example, in quantum electrodynamics (QED), there is no characteristic energy scale, and intermediate states can lead to terms with divergent integrals, such as

\[ \int_{m^2}^{\infty} \frac{dE}{E}. \]

The renormalization group addresses this problem of divergence by considering it to arise from the fact that there are infinitely many energy scales present in QED, all equally contributing to create such a divergent integral.

Thus, the renormalization group enables us to study the statistical continuum limit by equipping us to handle such divergences in a systematic way, much in the same way that the derivative has enabled us to study the ordinary continuum limit. The basic idea in renormalization group treatment of a problem is that length or energy scales become locally coupled to one another.

As an example [1], consider a magnet in which fluctuations of wavelength between 1000 and 2000 Å are predominantly affected by fluctuations in the ranges 500 to 1000 Å and 2000 to 4000 Å. One soon finds that a cascade effect results, as the 1 to 2 Å range influences the 2 to 4 Å range and the 2 to 4 Å range influences the 4 to 8 Å range, etc. Because of this cascade, amplification and deamplification take place in certain phenomena as one moves up through the length scales. For example, a small change in temperature will produce little effect on the 1 to 2
Å scale, which produces a slightly larger effect on the 2 to 4 Å scale, which produces a slightly larger effect on the 4 to 8 Å scale, until finally the change is macroscopic for large wavelengths. To illustrate deamplification, consider two magnetic materials that have significantly different atomic structures. The effect of the difference in the atomic structures usually decreases as one moves up in length scales, until the difference is finally unnoticeable at sufficiently large size. This is the basis of the universality hypothesis, which states that classes of different substances can display the same critical behavior.

The process of renormalization group analysis can be summarized as follows [1]: First, one must isolate a particular step in the cascade—i.e., some transformation that takes place as one moves from one length or energy scale to the next. Second, each step in the cascade results in an effective Hamiltonian for the scales yet to be solved. Scaling has been successfully achieved when the effective interaction remains unchanged after each step, meaning that one has arrived at a fixed point of the transformation. Third, one carries out the same cascade iterations for slightly different initial conditions, giving a set of amplification and deamplification parameters that are the eigenvalues of a version of the iteration obtained by linearizing about a fixed point. We shall see how each of these steps plays out specifically in the treatment of the Anderson problem.

As we shall see, a major application of the renormalization group is to solve the desired transformations numerically with a computer, which is how we shall approach the Anderson problem.

II. Description of the Anderson Problem

The Anderson problem is the study of spin-$\frac{1}{2}$ magnetic impurities in a nonmagnetic metal, such as copper doped with iron or manganese impurities. At low temperature, the impurities have strong effects on the thermodynamic properties of the metal, caused by coupling between impurity electrons and conduction electrons. The conduction electrons exchange spin with the impurities when they scatter off of them, and, consequently, the electrons can no longer be treated as independent. Typically, one wants the concentration of the impurity to be small, on the order of 0.01%, so that impurity properties, such as the magnetic susceptibility, are linear in the impurity concentration, making it easy to find the susceptibility due to a single impurity. If the impurity concentration becomes too large, the impurities begin to couple ferromagnetically to each other, making it difficult to achieve linearity in the impurity properties. The Anderson problem is similar to the Kondo problem, except that the Anderson model includes the coupling of $d$-state electrons in the conduction band to $d$-state electrons of the impurity, which the Kondo model ignores.

If one defines a spin-spin coupling strength, $J$, and treats the Anderson problem as a perturbation expansion, one finds [1] a term in the susceptibility that goes as $J^2 \ln(D/k_B T)$, where
\(D\) is the maximum electron energy, \(k_B\) is Boltzmann’s Constant, and \(T\) is the temperature. As \(T \to 0\), this term diverges. As in the case of QED, the appearance of this divergence can be explained to be due to a loss of a characteristic energy scale, resulting in a cascade. For a metal that obeys Fermi liquid theory, the characteristic energy scale is the Fermi energy, \(E_F\), arising from a delta function in the derivative of the electron energy distribution:

\[
\left. \frac{\partial n}{\partial E} \right|_{E=E_F} = X \delta(E-E_F).
\]

However, in a non-Fermi liquid, such as a metal with Anderson impurities, \(X = 0\), and the characteristic energy scale is lost, creating the cascade, which will be illustrated later. Thus, this is a perfect candidate for renormalization group treatment, in which we shall seek to define a renormalization group transformation and a sequence of effective Hamiltonians to treat the cascade in steps.

### III. Development of the Anderson Hamiltonian into a Discretized Form

In this section we will develop the Anderson Hamiltonian and begin making simplifications to the problem, arriving at a discretized form that will enable us to begin the renormalization group treatment. We begin with the original Anderson Hamiltonian \([2]\), which consists of, as grouped below, a conduction term, an impurity term, and a hybridization term \([3]\):

\[
H_A = \sum_{k} \varepsilon_k c_{k\uparrow}^\dagger c_{k\uparrow} + \left( \varepsilon_d c_{d\uparrow}^\dagger c_{d\uparrow} + U (c_{d\uparrow}^\dagger c_{d\uparrow})(c_{d\downarrow}^\dagger c_{d\downarrow}) \right) +
\sum_{k} \left( V_{kd} c_{d\uparrow} c_{d\uparrow} + V_{kd}^* c_{d\downarrow} c_{d\downarrow} \right),
\]

where all energies are measured with respect to the Fermi level \((\varepsilon = E - E_F)\) and repeated spin indices \((\mu, \text{in this case})\) are implicitly summed over. (Note that both of these conventions will remain in place for the rest of this paper.) The \(c_{k\mu} (c_{k\mu}^\dagger)\) operators are standard fermion annihilation (creation) operators of momentum \(\vec{k}\) and spin \(\mu\), obeying the anticommutation relations:

\[
\{c_{k\mu}, c_{\tilde{k}\mu}^\dagger\} = \delta_{\mu\nu} \delta^{(3)}(\vec{k} - \vec{\tilde{k}})
\]

\[
\{c_{k\mu}, c_{\tilde{k}\mu}\} = 0
\]
Our Hamiltonian can be rewritten as

\[
H_A = -\frac{1}{2} U + \sum_k \varepsilon_k c_{k\mu}^\dagger c_{k\mu} + \left( \varepsilon_d + \frac{1}{2} U \right) c_{d\mu}^\dagger c_{d\mu} + \frac{1}{2} U \left( c_{d\mu}^\dagger c_{d\mu} - 1 \right)^2 \\
+ \sum_k \left( V_{kd} c_{k\mu}^\dagger c_{d\mu} + V_{kd}^* c_{d\mu}^\dagger c_{k\mu} \right)
\]

which will be easier to simplify.

To simplify \( H_A \), we first assume that \( \varepsilon_k \) and \( V_{kd} \) are only functions of the magnitude of \( \vec{k} \). We also assume that the entire Fermi surface is contained inside a single conduction band ranging in energy from \(-D \leq \varepsilon \leq D\). These assumptions mean that we may use a set of spherical waves centered on the impurity site as a basis and that the impurity will only couple to \( s \)-wave electrons. We will label these states by energy instead of momentum, which will allow us to write the Hamiltonian in terms of electron creation and annihilation operators with the continuous label \( \varepsilon \), as in the equation below, thus making our summations into integrals from \(-D\) to \(D\).

Dropping the constant term, our Hamiltonian is now

\[
H_A = \int_{-D}^{D} \varepsilon a_{\varepsilon\mu}^\dagger a_{\varepsilon\mu} d\varepsilon + \left( \varepsilon_d + \frac{1}{2} U \right) c_{d\mu}^\dagger c_{d\mu} + \frac{1}{2} U \left( c_{d\mu}^\dagger c_{d\mu} - 1 \right)^2 \\
+ \int_{-D}^{D} d\varepsilon \left[ \rho(\varepsilon) \right]^{1/2} \left[ V_{d}(\varepsilon) a_{\varepsilon\mu}^\dagger c_{d\mu} + V_{d}^*(\varepsilon) c_{d\mu}^\dagger a_{\varepsilon\mu} \right]
\]

where \( \rho(\varepsilon) \) is the one-electron density of states per spin, \( V_{d}(\varepsilon) \) is \( V_{kd} \) from equation (2), and \( a_{\varepsilon\mu}^\dagger (a_{\varepsilon\mu}) \) is a creation (annihilation) operator of an electron in an \( s \)-wave state of energy \( \varepsilon \), which satisfies the anticommutation relations

\[
\{ a_{\varepsilon\mu}^\dagger, a_{\varepsilon'\mu'} \} = \delta_{\mu\mu'} \delta(\varepsilon - \varepsilon') \\
\{ a_{\varepsilon\mu}, a_{\varepsilon'\mu'} \} = 0
\]

We further simplify the Hamiltonian by replacing \( \rho(\varepsilon) \) and \( V_{d}(\varepsilon) \) with their values at the Fermi energy. Let us also define a dimensionless energy \( k \equiv \varepsilon / D \) and a corresponding annihilation operator \( a_{k\mu} = \sqrt{D} a_{\varepsilon\mu} \), which satisfies \( \{ a_{k\mu}^\dagger, a_{k'\mu'} \} = \delta_{\mu\mu'} \delta(k - k') \). Note that \( k \) will range from \(-1\) to \(1\), with \( k = 0 \) corresponding to the Fermi energy in the middle of the band. Let
us also define a constant $\Gamma = \pi \rho(\mathcal{E}_d) V_d(\mathcal{E}_d)^2$ for convenience. The Anderson Hamiltonian now takes the form

$$
\frac{H_A}{D} = \int dk \left[ \frac{1}{2} \left( \mathcal{E}_d + \frac{1}{2} U \right) c_{d\mu}^\dagger c_{d\mu} + \frac{1}{2} U D \left( c_{d\mu}^\dagger c_{d\mu} - 1 \right)^2 + \left( \frac{\Gamma}{\pi D} \right)^{1/2} \int_{-1}^{1} \frac{1}{D} \left( a_{k\mu}^\dagger c_{d\mu} + c_{d\mu}^\dagger a_{k\mu} \right) \right].
$$

(5)

Our next step in rewriting the Anderson Hamiltonian is the most important, as it will enable us to begin the renormalization group procedure. We begin by dividing up the dimensionless $k$-space using a logarithmic discretization. We choose a dimensionless parameter $\Lambda > 1$ and divide up the region $[-1, 1]$ into intervals defined by $\Lambda^{-n}$ for integer $n > 0$, as illustrated in Figure 1. Using this division, we define the $n$th interval to be $[\Lambda^{-n}, \Lambda^{-n+1}]$. Thus, the intervals become successively smaller with increasing $n$, and we have the series of energy scales that will be needed in the renormalization group treatment.

Using this discretization parameter, we define a complete set of spherical orthonormal wave functions (the Kondo basis) centered about the impurity:

$$
\psi_{np}(k) = \begin{cases} 
\frac{\Lambda^{n/2}}{(1-\Lambda^{-1})^{1/2}} \exp(i\omega_p pk) & \text{for } \Lambda^{-n} \ll k \ll \Lambda^{-n-1} \\
0 & \text{otherwise}
\end{cases},
$$

(6)

where $n = 0, 1, 2, \ldots$ labels the interval in which $\psi_{np}(k)$ is contained, the integer $p$ is the Fourier harmonic index ($p$'s physical relevance is unimportant since we will soon drop it), and $\omega_p$ is the fundamental Fourier frequency of the $n$th interval, given by

$$
\omega_n = \frac{2\pi}{1 - \Lambda^{-n}}.
$$

(7)

This basis of states is useful since it gives emphasis to those states that have the largest direct or indirect interaction with the impurity [1]. As $n$ increases, the radius of the $n$th state
increases, surrounding the impurity like layers of an onion. These states also have a logarithmic energy scale given by our discretization parameter $\Lambda$. One can envision this energy scale with the following physical scenario [1]: With an excitation energy of order 1 eV, an electron buried deep beneath the Fermi surface can jump to an energy far above the Fermi surface. With an excitation of only order 0.1 eV, an electron closer to the Fermi surface can jump to an energy less above the Fermi surface. A third electron can be excited with an energy of order 0.01 eV, etc. Each of these possibilities contributes to a logarithmic energy scale as depicted in Figure 2. Since each of these energy scales is equally present in the system, they result in a cascade causing the divergence in $\chi$ mentioned in Section II.

We can now expand the electron creation and annihilation operators in terms of a set of discrete operators, trading the continuous label $k$ for the integer labels $n$ and $p$ we introduced in (6):

$$a_{k\mu} = \sum_{n,p} \left[ a_{np\mu} \psi_{np} (k) + b_{np\mu} \psi_{np}^* (k) \right]$$

with

$$a_{np\mu} \equiv \int_{-1}^{1} dk \psi_{np}^* (k) a_{k\mu},$$

$$b_{np\mu} \equiv \int_{-1}^{1} dk \psi_{np} (k) a_{k\mu}.$$
These new operators satisfy

\[ \{ a_{np\mu}, a_{np'\mu'}^\dagger \} = \{ b_{np\mu}, b_{np'\mu'}^\dagger \} = \delta_{nn'} \delta_{\mu\mu'} \]  

(10)

with all other anticommutators zero.

We can now use the results

\[
\begin{align*}
\int_{-1}^{1} k a_{k\mu}^\dagger a_{k\mu} dk &= \frac{1}{2} (1 + \Lambda^{-1}) \sum_{np} \Lambda^{-n} \left( a_{np\mu}^\dagger a_{np\mu} - b_{np\mu}^\dagger b_{np\mu} \right) + \\
&\quad \frac{1 - \Lambda^{-1}}{2\pi i} \sum_{n, p\neq p'} \frac{\Lambda^{-n}}{p' - p} \left( a_{np\mu}^\dagger a_{np'\mu'}^\dagger - b_{np\mu}^\dagger b_{np'\mu'}^\dagger \right) \exp \left( \frac{2\pi i (p' - p)}{1 - \Lambda^{-1}} \right) \\
\int_{-1}^{1} a_{k\mu} dk &= (1 - \Lambda^{-1})^{1/2} \sum_{n} \Lambda^{-n/2} \left( a_{n0\mu} + b_{n0\mu} \right)
\end{align*}
\]  

(11)

to express the Anderson Hamiltonian (5) in terms of the new discretized operators. In doing so, we see that the impurity operators (the \( c_d \)'s) only couple to discretized operators that have \( p = 0 \). Thus, to a first approximation, we can ignore terms with \( p \neq 0 \). Physically, this approximation states that we are only going to consider electrons that are either near to the impurity in position space or near to the Fermi surface in momentum space [1]. This works out well, since at low temperatures, only electrons near the Fermi surface can become excited. This approximation does neglect terms in the Hamiltonian that couple operators that have \( p = 0 \) to operators that have \( p \neq 0 \). The strength of this coupling, and thus the error due to our approximation, is given by [1]

\[
\int_{-1}^{1} (k - k_n) \psi_{np}^\dagger (k) \psi_{n0} (k) dk ,
\]  

(12)

where \( k_n \) is the average value of \( k \) in the \( n \)th interval. For \( \Lambda \) near 1, \( (k - k_n) \) is small, and so the approximation is valid. It can be shown that this approximation works well for \( \Lambda \) as large as 3 [2].

Before we rewrite the Hamiltonian, let us define another operator

\[
f_{0\mu} = \left[ \frac{1}{2} (1 - \Lambda^{-1}) \right] \sum_{n=0}^{\infty} \Lambda^{-n/2} \left( a_{n\mu} + b_{n\mu} \right),
\]  

(13)

where we have dropped the label \( \rho \) from the discretized operators. (The subscript "0" on the new operator will become useful later.)
This new operator satisfies

\[ \{ f_{0\mu}, f_{0\mu}^\dagger \} = \delta_{\mu\mu'} \, . \quad (14) \]

Dropping the label \( p \) and inserting our new operator, the discretized Anderson Hamiltonian is

\[
\frac{H_A}{D} = \frac{1}{2} (1 - \Lambda^{-1}) \sum_{n=0}^{\infty} \Lambda^{-n} \left( a_{n\mu}^\dagger a_{n\mu} - b_{n\mu}^\dagger b_{n\mu} \right) + \frac{1}{D} \left( \epsilon_d + \frac{1}{2} U \right) c_{d\mu}^\dagger c_{d\mu} + \\
\frac{1}{2 D} \left( c_{d\mu}^\dagger c_{d\mu} - 1 \right)^2 + \left( \frac{2 \Gamma}{\pi D} \right)^{1/2} \left( f_{0\mu}^\dagger c_{d\mu} + c_{d\mu}^\dagger f_{0\mu} \right) \, .
\quad (15)\]

By transforming from the continuum Hamiltonian to the discretized Hamiltonian, we have gone from electrons with all possible energies between \(-1\) and \(1\) to electrons with a discrete set of energies \( \{ \pm \Lambda^n \} \). However, energies close to the Fermi surface \((k = 0 \text{ in Figure 1})\) will be well sampled, which works out well since these are the levels that determine the low-temperature behavior. We also note that as \( \Lambda \to 1 \), we recover the continuum limit (5).

We have one final step to take before we can apply the renormalization group techniques, which is to transform \( H_A \) into what is called a “hopping Hamiltonian.” To do this, we make a unitary transformation (as described in [2]) from the current set of discretized operators \((a_{n\mu}, b_{n\mu})\) to another orthonormal set \((f_{n\mu})\), with \( f_{0\mu} \) given as before. This will result in coupling \( f_{n\mu} \) operators of different \( n \). We will minimize this coupling by choosing a transformation such that only nearest-neighbor coupling takes place (i.e., \( f_{n\mu} \) only couples to \( f_{(n \pm 1)\mu} \)).

For convenience, let us define a set of constants:

\[ \xi_n = \left( 1 - \Lambda^{-n-1} \right) \left( 1 - \Lambda^{-2n-1} \right)^{1/2} \left( 1 - \Lambda^{-2n-3} \right)^{-1/2} \xrightarrow{n \to \infty} 1. \quad (16) \]

The discretized hopping Hamiltonian is thus

\[
\frac{H_A}{D} = \frac{1}{2} (1 - \Lambda^{-1}) \sum_{n=0}^{\infty} \Lambda^{-n/2} \xi_n \left( f_{n\mu}^\dagger f_{(n+1)\mu} + f_{(n+1)\mu}^\dagger f_{n\mu} \right) + \frac{1}{D} \left( \epsilon_d + \frac{1}{2} U \right) c_{d\mu}^\dagger c_{d\mu} + \\
\frac{1}{2 D} \left( c_{d\mu}^\dagger c_{d\mu} - 1 \right)^2 + \left( \frac{2 \Gamma}{\pi D} \right)^{1/2} \left( f_{0\mu}^\dagger c_{d\mu} + c_{d\mu}^\dagger f_{0\mu} \right) \, .
\quad (17)\]
We are now ready to examine this Hamiltonian using the renormalization group techniques.

IV. The Renormalization Group in Action: Iterative Diagonalization

The basic idea of the renormalization group approach to the Anderson problem is to begin by considering only the impurity and the innermost electron state \( n = 0 \) in the Kondo basis (6). One then adds on the terms involving the second state \( n = 1 \) and solves that system, and continues to add on each successive state and solve that physical system. This involves solving for the eigenvalues at smaller and smaller energy scales as depicted in Figure 2, thus treating the energy scale cascade in steps.

To do this, we define a set of dimensionless constants for convenience

\[
\begin{align*}
\delta_d &\equiv \left( \frac{2}{1 + \Lambda^{-1}} \right) \frac{1}{D} \left( \epsilon_d + \frac{1}{2} U \right) \\
\tilde{U} &\equiv \left( \frac{2}{1 + \Lambda^{-1}} \right) \frac{U}{2D} \\
\Gamma &\equiv \left( \frac{2}{1 + \Lambda^{-1}} \right)^2 \frac{2\Gamma}{\pi D}
\end{align*}
\]

and define a series of dimensionless Hamiltonians, \( H_N (N = 0, 1, 2, \ldots) \), as

\[
H_N \equiv \Lambda^{(N-1)/2} \sum_{n=0}^{N-1} \Lambda^{-n/2} \xi_n \left( f_{n\mu} \dagger f_{(n+1)\mu} + f_{(n+1)\mu} \dagger f_{n\mu} \right) + \delta_d c_{d\mu} \dagger c_{d\mu} + \tilde{U} \left( c_{d\mu} \dagger c_{d\mu} - 1 \right)^2 + \Gamma^{1/2} \left( f_{0\mu} \dagger c_{d\mu} + c_{d\mu} \dagger f_{0\mu} \right).
\]

We note that we can recover the original Hamiltonian with

\[
H_A = \lim_{N \to \infty} \left[ \frac{1}{2} \left( 1 + \Lambda^{-1} \right) D \Lambda^{-(N-1)/2} H_N \right].
\]

Thanks to our definition of \( f_{n\mu} \), these Hamiltonians obey a recursion relation

\[
H_{N+1} = \Lambda^{1/2} H_N + \xi_N \left( f_{N+1\mu} \dagger f_{(N+1)\mu} + f_{(N+1)\mu} \dagger f_{N+1\mu} \right),
\]

which will allow us to set up our renormalization group procedure. In the language of Section I, (21) is the transformation \( T \) that takes \( H_N \) into \( H_{N+1} \), leading us step by step through the cascade.
To solve for the eigenvalues of $H_N$, we set up an iterative diagonalization procedure [2] that we will organize into four steps. First, we let $|l, N\rangle$ denote the eigenstates of $H_N$ with energy $E(l,N)$, for $l = 0, 1, 2, \ldots, L_N$, letting $l = 0$ correspond to the ground state. (We will soon see what quantum numbers we should use to describe these states and will replace $l$ accordingly.) Each Hamiltonian $H_N$ will have $(L_N + 1) = 2^{(N+2)}$ states.

Second, we construct the following set of $4(1+L_N)$ orthonormal states:

$$
|1, l, N\rangle \equiv |l, N\rangle
$$

$$
|2, l, N\rangle \equiv f_{(N+1)\uparrow}^{-1} |l, N\rangle
$$

$$
|3, l, N\rangle \equiv f_{(N+1)\downarrow}^{-1} |l, N\rangle
$$

$$
|4, l, N\rangle \equiv f_{(N+1)\uparrow}^{-1} f_{(N+1)\downarrow}^{-1} |l, N\rangle
$$

(22)

These states provide a basis that spans the space of $H_{N+1}$.

Third, we compute the matrix elements of $H_{N+1}$ in the $|i,l,N\rangle$ basis, which turn out to be given by

$$
\langle i', i', N | H_{N+1} | i, l, N \rangle = \Lambda^{1/2} E(l, N) \delta_{ii'} \delta_{ll'} + \xi_N \left( \langle i', N | f_{N\mu}^{-1} | l, N \rangle \langle i', i', N | f_{(N+1)\mu}^{-1} | l, N \rangle + \langle i', i', N | f_{(N+1)\mu}^{-1} | i, l, N \rangle \langle l', N | f_{N\mu}^{-1} | l, N \rangle \right).
$$

(23)

Once we have all the matrix elements of $H_{N+1}$, the fourth and final step is to diagonalize $H_{N+1}$ to get its $L_{N+1}$ eigenstates, $|l, N + 1\rangle$, of energy $E(l,N+1)$. We then repeat the process to solve for $H_{N+2}$.

We see from (23) that what we need to know in order to carry out this iterative diagonalization are the energy levels $E(l,N)$ and the matrix elements $\langle i', N | f_{N\mu}^{-1} | l, N \rangle$ for some starting Hamiltonian, usually $H_0$, and we may, in theory, iterate up to arbitrarily large $N$.

Of course, running these iterations soon becomes rather impractical, since the number of states for each Hamiltonian is of the order $2^{(N+2)}$. After the first few iterations, the calculations becomes too cumbersome and computationally expensive. However, there are a few steps we can take to curb these impracticalities.

First, we can exploit several symmetries of the iterative Hamiltonian (19) to make the work of diagonalization easier [2]. Our $H_N$, we see, conserves spin and electron number (or
charge), defined, respectively, as

\[
\bar{S}_N = \frac{1}{2} \sum_{n=0}^{N} f_{nP}^\dagger \sigma_{\mu\nu} f_{mN}^\dagger + \frac{1}{2} c_{d\mu}^\dagger \sigma_{\mu\nu} c_{d\mu}^\dagger,
\]

\[
Q_N = \sum_{n=0}^{N} \left( f_{nP}^\dagger f_{mN}^\dagger - 1 \right) + \left( c_{d\mu}^\dagger c_{d\mu}^\dagger - 1 \right),
\]

where \( \sigma_{\mu\nu} \) represents the Pauli spin matrices. Thus, we may label the states \( |l, N \rangle \) with quantum numbers \( Q, S \) and \( m_s \). This also means that each of our iterative Hamiltonians will reduce to block diagonal form, since they will not have matrix elements between states of different values of \( (Q, S, m_s) \), and each matrix block may be diagonalized individually. This feature opens up the possibility for utilizing a parallel processing algorithm in which computers running in parallel could each solve a subset of the Hamiltonian blocks.

If we work with the symmetric case, for which \( \epsilon_{\mu} = -\frac{1}{2} U \) and thus \( \hat{\delta} = 0 \), our \( H_N \) simplifies and it will also observe particle-hole symmetry, given by the transformation

\[
f_{nP} \to (-1)^n f_{nP}^\dagger, \quad c_{d\mu} \to -c_{d\mu}^\dagger.
\]

If we apply this transformation to (24), we see that it takes \( Q_N \) into \(-Q_N\). Thus, the state with quantum numbers \( (Q, S, m_s) \) will have the same energy as the state with quantum numbers \((-Q, S, m_s)\), and we only need to diagonalize for states with \( Q \geq 0 \).

Even with these tricks from symmetry properties, we still find it impractical to calculate every eigenstate for large \( N \). But it is also unnecessary: Since we are interested in low-temperature behavior, we only need the lowest energy eigenstates of each \( H_N \). Going back to Figure 2, if the temperature is sufficiently small, we can ignore energy excitations—and thus eigenstates of \( H_N \)—above a certain level. Typically, one chooses a maximum number of states to retain at the end of each iteration, say 1000 or 2000, and then keeps that many of the lowest-lying states. However, this state truncation will produce an error in the calculation of thermodynamic properties and the matrix elements of \( H_{N+1} \). To make matters worse, this error will become larger as \( \Lambda \to 1 \), which is the continuum limit that we want. Thus, the choice of \( \Lambda \) and the number of states kept at the end of each iteration must be based on a balance of desired accuracy and computing costs.

Now that we have established our iterative diagonalization procedure, we shall discuss the nature of the fixed points of our sequence of Hamiltonians (19).
V. Fixed Points of the Renormalization Group Transformation

As stated in Section I, we are interested in investigating fixed points of the renormalization group transformation—i.e., Hamiltonians $H^*_N$ that the transformation $T$ (as given by (21)) leaves invariant: $T[H^*_N] = H^*_N$. In terms of our iterative procedure of the previous section, a fixed point is one at which the transformation $T$ will take the energy eigenvalues of $H^*_N$ and the matrix elements of the $f_N$ operator into themselves. It turns out [2], however, that $T$ does not have any such fixed points, but $T^2$ does. Thus, we will be looking for the energy levels and matrix elements to repeat at the end of every other step in the iterative procedure. It can be shown [2] that the Hamiltonian for a system with no impurity, given by

$$H^0_N \equiv \Lambda^{(N-1)/2} \sum_{n=0}^{N-1} \Lambda^{-n/2} \xi_n \left( f_{n\mu}^\dagger f_{(n+1)\mu} + f_{(n+1)\mu}^\dagger f_{n\mu} \right),$$  \hspace{1cm} (26)

will lead to two fixed points of $T^e$, one for odd $N$ and one for even $N$, which we shall denote as $H^*$ and $\hat{H}^*$, respectively. For the symmetric case, $\delta_\mu = 0$, we find [2] that there are three classes of fixed points for the transformation $T^e$, each with one fixed point for odd $N$ and one for even $N$, which can all be described in terms of $H^*$ and $\hat{H}^*$.

First, if we set $\tilde{\Gamma} = \tilde{U} = 0$, and thus turn off the effects of the impurity’s spin, we get two free-orbital fixed points. We denote these free-orbital Hamiltonians as $H^*_{FO} (\hat{H}^*_{FO})$ for odd (even) $N$, which are given by $H^* (\hat{H}^*)$ plus a free-impurity orbital of zero energy.

Second, if we let $U$ become much larger than all other energies, we find two local-moment fixed points, denoted $H^*_{LM} (\hat{H}^*_{LM})$ for odd (even) $N$. In this situation, the impurity is no longer interacting with the conduction electrons and it reduces to a simple local spin-$\frac{1}{2}$ moment. Thus, $H^*_{LM} (\hat{H}^*_{LM})$ is given by $H^* (\hat{H}^*)$ plus a term for a local spin-$\frac{1}{2}$ moment.

Finally, if we let $\Gamma$, the strength of the electron-impurity interaction, become much larger than all other energies, we get two strong-coupling fixed points, denoted $H^*_{SC} (\hat{H}^*_{SC})$ for odd (even) $N$. In this case, the impurity and the innermost conduction electron become so strongly coupled that they cease to interact with the other electrons. Since the innermost electron is now subtracted off, $H^*_{SC} (\hat{H}^*_{SC})$ is simply given by $\hat{H}^* (H^*)$. We note that since the system is now “missing” an electron, the odd and even fixed points have swapped Hamiltonians.

As an aside, one may be tempted to think that this last scenario could potentially be the source of electron crystallization—that the strong coupling between the electrons and the impurities throughout the metal could cause each electron to localize into its own small range of position space, forming a crystal. However, in order for this to happen, each electron would have to have its own impurity to become coupled to, and so the density of impurities would have to equal the density of conduction electrons. Since the density of electrons is usually is usually on
the order of the density of non-magnetic ions, this would destroy the assumption that the impurity concentration is low. What one typically finds as one iterates $H_N$ up to higher $N$ is that there are ranges of $N$ in which $H_N$ becomes close to one of these fixed points. We will see this come about in the numerical results of Section VII. We are now ready to discuss the calculation of the magnetic susceptibility and then move on to the numerical results.

VI. Magnetic Susceptibility

The calculation of the thermodynamic properties of the impurity will involve evaluating the operator $\exp(-\beta H_A)$, where $\beta = (k_B T)^{-1}$. To do this, let us define a similar iterative operator, $\exp(-\bar{\beta}_M H_M)$, where $H_M$ is the iterative Hamiltonian given by Equation (19)—our reason for trading $N$ for $M$ will be seen shortly—and

$$\bar{\beta}_M \equiv \beta_D \frac{1}{2} \left(1 + \Lambda^{-1}\right) \Lambda^{-(M-1)/2}$$

(27)

is a dimensionless temperature parameter. We then have

$$\exp(-\bar{\beta}_M H_M) \xrightarrow{M \to \infty} \exp(-\beta H_A).$$

(28)

The impurity contribution to the magnetic susceptibility is thus

$$\chi_{\text{imp}}(T) = \frac{(g \mu_B)^2}{k_B T} \lim_{M \to \infty} \left[ \frac{\text{Tr} S^2_M \exp(-\bar{\beta}_M H_M)}{\text{Tr} \exp(-\bar{\beta}_M H_M)} - \frac{\text{Tr} S^0_M \exp(-\bar{\beta}_M H^0_M)}{\text{Tr} \exp(-\bar{\beta}_M H^0_M)} \right],$$

(29)

where $g$ is the electron $g$-factor, $\mu_B$ is the Bohr Magneton, and $H^0_M$ is the Hamiltonian with no impurity present as given in (26). Similarly,

$$\bar{S}^0_M = \frac{1}{2} \sum_{n=0}^{M} f^+_n \bar{\sigma}_{\mu v} f^v_n$$

(30)

is the spin operator with no impurity present. If we use $Q$, $S$, and $m_s$ as labels for our states as mentioned in Section IV, then the traces in (29) reduce to simple sums over $Q$, $S$, and $m_s$.

It can be shown [2] that if we only take $M$ up to some finite $N$, instead of to infinity, the error incurred in the calculation of $\chi_{\text{imp}}$ is only of order $\bar{\beta}_N / \Lambda$. Thus, in order to evaluate $\chi_{\text{imp}}$ at
a desired low temperature $T$, we only have to choose a small number $\beta$ and an $N$ such that $\beta_N = \beta$, and then run our iterative diagonalization procedure up to $M = N$. Thus, running the sequence of Hamiltonians, $H_m$, from $M = 0$ to $N$ allows us to compute $\chi_{\text{imp}}$ (and other thermodynamic properties) to an accuracy of order $\beta_N / \Lambda$ for a sequence of temperatures $T_N(\beta)$, given by $\beta_N = \beta$:

$$T_N(\beta) = \frac{D}{2k_B \beta} \left(1 + \Lambda^{-1}\right) \Lambda^{-\left(N-1\right)/2}.$$  \hspace{1cm} (31)

This logarithmic temperature scale provides a rough estimate of the accuracy of the renormalization group approach, since we can choose different values of $\beta$ and $N$ that will have the same value of $T_N(\beta)$ and compare their results.

We are now ready to examine the numerical results of our iterative procedure.

### VII. Numerical Results

In closing, we will take a look at some of the numerical results obtained from the method outlined in this paper. Note that all of these results are for the symmetric case, $\delta_d = 0$. The first two sets, Figures 3 and 4 [2], show the development of the lowest-lying energy levels as a function of $N$. Since we are looking for fixed points of the transformation $T^e$, the graphs only display the energies for odd $N$. Each curve represents the energy levels for a given eigenstate as it evolves with $N$. The vertical axes are labeled in terms of the set of energies $(\tilde{\eta}_a^*, \tilde{\eta}_a)$, which are the eigenenergies of the fixed points $H^*$ and $\hat{H}^*$ mentioned in Section V. In Figure 3, we see that the energy levels for $5 < N < 15$ remain close to the free-orbital fixed point, for $23 < N < 51$ they remain close to the local moment fixed point, and for $61 < N$ they remain close to the strong coupling fixed point. In Figure 4, we see similar behavior, except that the energy levels go straight from the free-orbital fixed point ($5 < N < 15$) to the strong-coupling fixed point ($25 < N$). We are already beginning to see that only the strong-coupling fixed point is a stable fixed point.

The second two sets of results, Figures 5 and 6 [2], show the results for the susceptibility $\chi_{\text{imp}}$. The dashed curves are the universal susceptibility curves for the Kondo model, with the effective Kondo temperature marked with an arrow. The values $\rho\mu_{\text{SW}}$ are given by $-8\Gamma/(\pi U)$. In Figure 5, the curve labeled A corresponds to the energy levels in Figure 3, and we see that the susceptibility also tends to hover near one of the three fixed points (recall the logarithmic temperature scale that relates $T$ and $N$ (31)). We find the free-orbital regime has $T\chi_{\text{imp}} = 1/8$, the
Figure 3. Lowest-lying energy levels of $H_N$ for odd $N$ with $U/D = 10^{-3}$, $U/\pi \Gamma = 12.66$, and $\Lambda = 2.5$; axes labeled in terms of fixed-point energies of $H_{N'}$.

Figure 4. Lowest-lying energy levels of $H_N$ for odd $N$ with $U/D = 10^{-3}$, $U/\pi \Gamma = 1.013$, and $\Lambda = 2.5$; axes labeled in terms of fixed-point energies of $H_{N'}$.

Figure 5. Plots of $k_B T_{c_{imp}}$ vs. $\ln(k_B T/D)$, with plot A (B) the same physical scenario as Figure 5 (6).

Figure 6. Plots of $k_B T_{c_{imp}}$ vs. $\ln(k_B T/D)$, with $U/D = 0.5$, $U/\pi \Gamma = 5.629$ (A), 2.026 (B), and 1.013 (C).
local moment regime has $T_{\chi_{\text{imp}}} = 1/4$, and the strong coupling regime has $\chi_{\text{imp}}$ constant, making the curve linear in $T$. Similarly, the curve labeled B corresponds to the energy levels in Figure 4, and we see that the susceptibility goes straight from the free orbital ($T_{\chi_{\text{imp}}} = 1/4$) to the strong coupling regime ($\chi_{\text{imp}}$ constant). In Figure 6, we see similar behavior, noting that in curve C, there is no longer a free-orbital regime.

This behavior of $H_N$ "resting" near the various fixed points for different ranges of $N$ can be thought of in terms of the diagram depicted in Figure 7 [2]. If we associate each $H_N$ with effective energies $U_{\text{eff}}$ and $\Gamma_{\text{eff}}$, we can think of increasing $N$—going through the iterative diagonalization—as taking $H_N$ along the trajectories in the graph. As demonstrated in our numerical results, only $H_{\text{SC}}^*$ is a stable fixed point. It can be shown [2] that for every choice of $U$ and $\Gamma$ with $\Gamma \neq 0$, there is some critical $N_C$ such that for any $N > N_C$, $H_N$ will be close to the strong-coupling fixed point.

Consequently, there is a corresponding critical temperature $T_C$ such that for $T < T_C$, the impurity thermodynamic properties can be calculated by an approximate Hamiltonian built on $H_{\text{SC}}^*$. For $U \gg \Gamma$, $T_C$ is the Kondo temperature, $T_K(\Gamma, U)$. For $\Gamma \gg U$, $T_C$ is of the order of $\Gamma$. This behavior is illustrated in Figure 8 [2], showing the various fixed-point regimes for given $U$, $\Gamma$, and $T$. It should be noted that the boundaries between the three regimes are to be taken as approximate, since, as we can see in Figures 3 and 4, the transitions between the regimes are gradual rather than sharp.

These results illustrate well the principle of universality, a very important aspect of the renormalization group that was alluded to in Section I. In this situation, universality means that a wide variety of choices for $H_N$ for small $N$ will iterate up to approximately the same sequence of Hamiltonians for large $N$ [2]. For example, we chose to replace $\rho(\epsilon)$ and $V_d(\epsilon)$ by their values at the Fermi energy. It can be shown [2] that if we let them be slightly energy dependent, the

Figure 7. Evolution of $H_N$ with increasing $N$. Note that only $H_{\text{SC}}^*$ is a stable fixed point.

Figure 8. Illustration of the regimes of the fixed points. Note that the strong-coupling regime exists for any $\Gamma \neq 0$ and $U$ for $T < T_C$.
corrections to $H_n$—though they may be significant for small $N$—will not change the result that $H_n$ for large $N$ will approach $H^*_\text{sc}$.

VIII. Conclusions

We have seen that the techniques of the renormalization group provide an excellent method for analyzing the Anderson problem. By transforming the Anderson Hamiltonian appropriately, and introducing the key logarithmic energy discretization through the parameter $\Lambda$, we have shown that it is possible to regulate the divergence that would otherwise occur in impurity properties such as the susceptibility. This has proven to be an excellent example of the usefulness of the renormalization group in calculating physical phenomena. What remains to be done in future work is the task of making these computations more efficient and accurate.