Scattering approach to Impurity Thermodynamics

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Recently the authors developed a scattering approach that allows for a complete description of the steady-state physics of quantum-impurities in and out of equilibrium. Quantum impurities are described using scattering eigenstates defined *ab initio* on the open, infinite line with asymptotic boundary conditions imposed by the leads. The scattering states on the open line are constructed for integrable quantum-impurity models by means of a significant generalization of the Bethe-Ansatz which we call the Scattering Bethe-Ansatz (SBA). The purpose of the paper is to present in detail the scattering approach to quantum-impurity models and the SBA and show that they reproduce well-known thermodynamic results for several widely studied models: the Resonance Level model, Interacting Resonance Level model and the Kondo model. Though the SBA is more complex than the traditional Thermodynamic Bethe Ansatz (TBA) when applied to thermodynamical questions, the scattering approach (SBA) allows access to an array of new questions that cannot be addressed otherwise, ranging from scattering of electrons off magnetic impurities to nonequilibrium dynamics.

I. INTRODUCTION

Recent advances in nanotechnology have allowed extensive experimental study of quantum impurity systems out of equilibrium in controlled, tunable settings[1]. The impurities are typically realized as quantum dots, tiny islands of two-dimensional electron gas attached to leads via tunnel junctions. The number of electrons on the dot can be controlled using a gate voltage since the hopping of electrons is impeded by a large charging energy U. When there is an odd-number of electrons on the dot the upper-most energy level contains only a single, unpaired electron, which behaves effectively as an Anderson or Kondo impurity coupled to the two (or more) leads playing the role of electron baths. Applying a potential difference between the leads results in a current flowing across the dot. A wealth of new experimental data has been collected in recent years on quantum-impurities out of equilibrium in this setting including current vs voltage curves and nonequilibrium density of states (DOS) on the quantum dots[2]. Nonetheless, a comprehensive theoretical understanding of the physics of these models is lacking.

Quantum impurity systems are also the simplest examples of strongly correlated electron systems, wherein interactions between electrons are strong enough to result in new collective behaviors which require a new set of degrees of freedom for their description- the Kondo effect being a canonical example[3]. The strongly-correlated behavior is typically characterized by a low energy scale such as the Kondo temperature below which strong correlation physics dominates and perturbative descriptions break down. One of the most fascinating new frontiers in strongly-correlated systems is the study of such systems in out-of-equilibrium situations. Quantum impurities are an ideal experimental and theoretical setting for exploring the interplay between nonequilibrium- and strongly-correlated dynamics due to the relative simplicity of these models and the wealth of experimental data available.

New theoretical questions arise in this context. Do sufficiently large voltages suppress strong-correlations and thus kill the Kondo effect? Do new scales, such as the decoherence scale, arise? Does voltage effectively behave as a temperature? How should one handle intrinsically non equilibrium phenomena such as nonequilibrium particle and energy currents or entropy production. What is the effect of strong correlation the entropy production?

Currently, the most commonly used technique to treat quantum-impurities out of equilibrium is Keldysh perturbation theory[4]. The perturbative methods, however, are applicable only in the high voltage regime and break down precisely where strong correlations become important. As such, they are unable to answer the interesting questions proposed above. A variety of non-perturbative techniques have been developed in order to capture the strong correlation physics of quantum impurity models, mainly in the context equilibrium physics. These include renormalization group methods, techniques from bosonization and conformal field theory, and exact solutions using the Bethe-Ansatz[3]. Most of these methods are no longer applicable when the influence of nonequilibrium dynamics is comparable to the strong correlations in the problem. This highlights the need for new theoretical approaches that can probe the interesting non-perturbative regimes[5,6,7,8,9,10].

Recently we have introduced such a non-perturbative framework that allows the description of a steady state out-of-equilibrium quantum impurity system in terms of a time-independent scattering formulation[11]. A steady state ensues[12] when the system is *open*. Open systems must be defined directly on the infinite line to allow an in-flow and out-flow of electrons and energy from the system. The infinite volume limit, which needs to be taken *ab initio*, provides a dissipation mechanism. Under these circumstances the non-equilibrium steady state can be described by a scattering eigenstate of the full hamiltonian, an eigenstate defined on the infinite line with its asymptotic behavior specified at the incoming infinity. In most cases the asymptotic boundary conditions are determined by the electron leads[11].

We have subsequently also introduced a method, the Scattering Bethe Ansatz (SBA), to construct those scattering eigenstates on the infinite line for the Kondo model and other integrable impurity models. The traditional Bethe Ansatz, on the other hand, which has been extensively applied to these models, is defined with periodic boundary condition with periodicity L (with L subsequently sent to infinity). This approach is appropriate to *closed* systems and allows an efficient calculation of the thermodynamic properties of the systems. However, it does not give access to their scattering properties, nor to the non-equilibrium physics.

The scattering approach can also be applied under equilibrium conditions, when all baths are held at the same chemical potential, or in the case when only one lead is present. The purpose of this paper is to study the Scattering Approach under these simpler circumstances and confront it with the conventional approach which can also be applied here. We will show that the SBA reproduces known thermodynamical results for quantum-impurity models. Nonetheless, as mentioned above, the algebraic Bethe-Ansatz and its finite temperature counterpart the Thermodynamic Bethe Ansatz, prove technically easier when calculating thermodynamics of quantum-impurity models. The real advantage of the SBA is that it allows us to harness the power of integrability to explore new questions about electron S-matrices and T-matrices important for understanding quantum-mechanical coherence and dephasing due to magnetic impurities[13,14]. And, in a context which we will not further explore in this paper, SBA allows us to understand nonequilibrium steady-states in these models.

The paper is organized as follows. We start with a formal introduction to the scattering approach to quantum-impurity models and the scattering Bethe-Ansatz (SBA). Subsequently, we demonstrate our ideas on the Resonant Level model where the physics is particularly simple since the Hamiltonian is quadratic. Finally, we use the SBA to construct scattering states to reproduce well-known $T = 0$ equilibrium results for Interacting Resonant Level and Kondo models. We conclude the paper with some conjectures about the Kondo model that significantly simplify the calculation of some impurity properties.

II. THE SCATTERING FORMALISM

The basic idea underlying the scattering formalism is the observation that a quantum impurity can be viewed as a localized dynamical scatterer off which electrons from the attached leads or host metal scatter. The scattering changes the internal state of both the impurity and host electrons and leads to the generation of strong correlations. The standard procedure for treating such problems is to set-up an initial state with wavepackets that represent the incoming particles in the far past and evolve this initial state for a very long time with a time-evolution operator $U(t,t_o) = T\exp(-i\int_{t_o}^{t} H(t')dt')$ of the appropriate interacting field-theory; H is the Hamiltonian that describes the particles and dynamical scatterer - in this case the quantum impurity. As the impurity is local, the interaction switches off far away from the impurity and we can define 'in' or 'out' states by specifying the asymptotic behavior in the far past or the far future. Namely, the 'in' , respectively, 'out' states are eigenstates of the total Hamiltonian, satisfy the boundary conditions that they tend to plane waves representing free incoming particles in the $t \to -\infty$ and $t \to \infty$ limits respectively. The cross-section for a particular process is then obtained by calculating the overlap of the "in" state with an appropriate "out" state. A recent application of these ideas to quantum impurities is given in[15,16]. While scattering states are designed to allow access to the scattering properties of the system, they also allow calculation of the thermodynamic properties.

The Hamiltonian for a quantum impurity attached to a bath of free electrons is of the form:

$$H = H_0 + H_{\rm int} = \sum_{\alpha,\vec{k}} \epsilon_k \psi^\dagger_{\alpha\vec{k}} \psi_{\alpha\vec{k}} + H_{\rm int} \qquad (1)$$

with ϵ_k the full three-dimensional dispersion of the electrons and α denoting the internal degrees of freedom of the electrons. The term $H_{\rm int}$ describes the impurity and its interaction with the bath of electron. Examples include the Kondo interaction,

$$H_{\rm int} = J \sum_{a\vec{k}} \psi^\dagger_{a\vec{k}} \ (\vec{\sigma})_{aa'} \sum_{a'\vec{k'}} \psi_{a'\vec{k}'} \cdot \vec{S},$$

with $\vec{S}$ a localized spin representing the impurity, and the resonance level model (RLM),

$$H_{\rm int} = t \sum_{\vec{k}} (\ \psi^\dagger_{\vec{k}} d + h.c.) + \epsilon_d d^\dagger d,$$

describing a local level at energy ϵ_d which hybridizes with the bath electrons.

Standard manipulations[17] allow us to rewrite the Hamiltonian as chiral 1-d field theories. Since only the combination $\sum_{a\vec{k}} \psi^\dagger_{a\vec{k}}$ enters into the interaction we can rewrite the theory in terms of the field

$$\psi^\dagger_{\alpha\epsilon} = \int d^3k \ \delta(\epsilon_k - \epsilon) \psi^\dagger_{a\vec{k}}$$

as (D denotes the bandwidth, namely the cut-off)

$$H_0 = \int_{-D}^{D} d\epsilon \ \epsilon \ \psi^\dagger_{\alpha\epsilon} \psi_{\alpha\epsilon}$$

while the interaction terms take the form, $J\int d\epsilon \ \psi^\dagger_{a\epsilon} \ (\vec{\sigma})_{aa'} \int d\epsilon' \psi_{a;\epsilon'} \cdot \vec{S}$ or $t(\int d\epsilon \ \psi^\dagger_\epsilon d + h.c.) + \epsilon_d d^\dagger d$ for the Kondo or the IRLM Model respectively. Finally introducing a chiral fermion field

$$\psi^\dagger_\alpha(x) = \int_{-D}^{D} e^{i\epsilon x} \psi^\dagger_{\alpha\epsilon} \nu(\epsilon)^{-1/2}$$

the kinetic term becomes

$$H_0 = -i \int_{-D}^{D} dx\ \psi_\alpha^\dagger(x)\partial_x\psi_\alpha(x)$$

while the field enters locally into $H_{\rm int}$, in the form $\psi_\alpha^\dagger(0)$. As we are interested in the physics on energy scales much smaller than the cut-off D, we consider only universal results obtained in the limit $D \to \infty$.

Open vs Closed Boundary Conditions: The scattering approach to quantum impurity problems, by its very nature, is defined in infinite systems, *without* boundaries. Physically, this is equivalent to requiring that once incoming electrons scatter off the impurity they do not return and scatter off the impurity again. We refer to infinite size systems with no boundaries as "open systems". The infinite size of the electron bath assures that the host metal or lead is a good thermal bath. Real life systems are not infinite but possess boundaries; our treatment is valid as long as the return time for the electrons is much smaller than the system size. The infinite size of the system implies that scattering states are no longer normalizable and in particular, the Feynman-Hellman theorem no longer holds[18]. This will be important in understanding the results of later sections when we construct eigenstates for the IRLM and Kondo models.

In this open system framework the nature of the incoming particles that scatter off the impurity is specified by asymptotic boundary conditions. The incoming particles, far from the impurity, are eigenstates of the free-electrons Hamiltonian H_0 and any eigenstate of H_0 is a possible boundary condition describing what the incoming particles look like. Two different boundary conditions are of primary interest: (i) when the incoming particles are a Fermi sea, typically representing the host metal and (ii) when the incoming particles are a Fermi sea and an excited quasi-particle. The former allows for us to calculate thermodynamical properties from scattering while the latter allows us to compute, in principle, single particle S and T matrices. These boundary conditions are depicted in Figure 1.

Time Dependent and Time Independent Formalisms: $T = 0$: There are two different descriptions for scattering processes. In the time-dependent description, the interaction between the conduction electrons and quantum impurity is turned on in the far past, at $t = t_o$ and then adiabatically time-evolved using the Hamiltonian

$$H = H_o + e^{\eta t} H_{\rm int}\theta(t - t_o), \tag{2}$$

with H_o describing the free electron bath and H_{int} the interactions between the quantum impurity and the incoming electrons, i.e., between the dot and the leads. Before $t = t_o$ the quantum impurity is decoupled from the electron bath and the system is described by an asymptotic boundary condition, an eigenstate of H_0 which we denote $|\Phi_o\rangle$ (at $T > 0$ the system is described by some density matrix ρ_o describing decoupled leads and the dot).

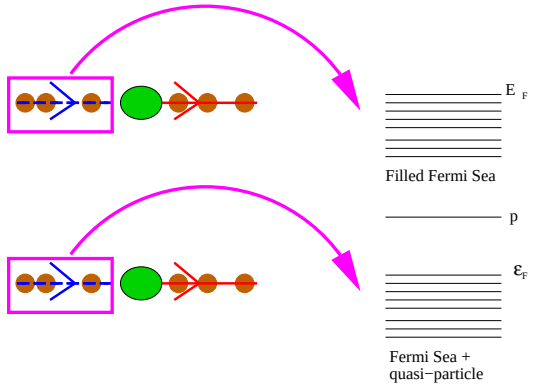

FIG. 1: The incoming particles in the chiral picture correspond to the particles on the left of the impurity and the outgoing scattered particles are on the right. We take the convention that the impurity is at $x = 0$. Using this convention, incoming particles are located on the negative x-axis, $x < 0$, and outgoing particles to the positive x-axis, $x > 0$. We typically consider two types of open boundary conditions for incoming particles. In the first, the incoming particles describe a filled Fermi sea. This is useful for calculating thermodynamics. In the second, the incoming particles are a Fermi sea and an excited quasi-particle. This allows us to calculate the single-particle S and T matrices.

At later times, as the baths and the quantum-impurity evolve, the interaction is turned on adiabatically[28] from the state $|\Phi_o\rangle$ under the action of the time evolution operator

$$\begin{aligned} |\Psi(t)\rangle &= U(t, t_o)|\Phi_o\rangle \\ U(t, t_o) &= T\{\exp\left(-i \int_{t_o}^{t} dt' H(t')\right)\} \end{aligned} \tag{3}$$

We now wish to establish that a steady-state ensues after sufficiently long time- long enough that all transients die out. For this purpose one must show that the limit $t_o \to -\infty$ exists, free of infra-red divergences. This has been shown to be the case for the Kondo model[12] under the condition that the infinite volume limit is taken first, i.e. the system is open and the impurity is coupled to good thermal baths. The "openness" of the system provided the dissipation mechanism necessary for the steady state, allowing the high-energy electrons to relax and escape to infinity. The adiabatic limit $\eta \to 0$ is taken last, allowing the smearing of the bath levels (level separation $\delta \sim 1/L$ to take place turning the poles in the Green's function into a cut).

Under these circumstances $|\Psi(t)\rangle$ become time-independent and describes a time independent eigenstate which we denote $|\Psi\rangle_s$. Thus, we can also describe our state in a time-dependent picture. In the time-independent picture time is traded for space and - for the chiral unfolded picture- the far past corresponds to incoming particles located at distances $x \ll 0$ and the far future to outgoing particles located at $x \gg 0$. (see Figure 1). Under both equilibrium and non-equilibrium

conditions (e.g. coupling to baths at different chemical potentials), the expectation value of any operator $\hat{O}$

$$\langle \hat{O} \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle_s}{\langle \Psi | \Psi \rangle_s} \tag{4}$$

is time independent.

A stronger conclusion can be deduced which is central to our construction: the state $|\Psi(0)\rangle = |\Psi\rangle_s$ becomes, by the Gellman-Low theorem[19], an eigenstate of the full Hamiltonian H, specified by the initial condition $|\Phi_o\rangle$ that describes the electrons in the far past ($x \ll 0$). In other words , the state $|\Psi\rangle_s$ is a scattering eigenstate of the full hamiltonian $H = H_0 + H_{\rm int}$, satisfying the Lippman-Schwinger equation,

$$|\Psi\rangle_s = |\Phi_o\rangle + \frac{1}{E - H_0 \pm i\eta} H_{\rm int} |\Psi\rangle_s \tag{5}$$

with $|\Phi_o\rangle$ - the incoming state playing the role of a boundary condition imposed asymptotically. The scattering state $|\Psi\rangle_s$ can be viewed as consisting of incoming particles (commonly taken to be a bath of free electrons) described by $|\Phi_o\rangle$, and of scattered outgoing particles given by the second term in the above equation. Once again two elements are required to fully determine the system: a hamiltonian, H, and a boundary condition, $|\Phi_o\rangle$, which describes the incoming scattering state far from the impurity. Note that previously, in the time-dependent picture, $|\Phi_o\rangle$ played the role of an initial condition rather than a boundary condition. As the impurity is short ranged the scattering state $|\Psi\rangle_s$ must reduce to the eigenstate $|\Phi_o\rangle$ when all the particles are far to the left of the impurity. This gives a prescription for calculating scattering eigenstates for quantum-impurity problems. We must construct an eigenstate of the full Hamiltonian H with the requirement that when all the electrons are to the left of the impurity the eigenstate reduces to a prescribed eigenstate of H_0 describing the free decoupled two baths and the impurity. It is worth emphasizing that we never explicitly solve (5). Instead, we directly construct eigenstates of the full-Hamiltonian with $|\Psi\rangle_s$ that are of the form described above.

Scattering formalism at finite Temperatures: The above discussion can be generalized to finite temperatures. Once again there are two equivalent frameworks for quantum-impurity problems, a time-dependent and time-independent. In the former, we proceed as in the zero temperature case. We consider the quantum impurity and the baths to be decoupled in the far past, at $t = t_o \to -\infty$, adiabatically turning on the coupling. The Hamiltonian is again given by (2). The change from zero temperature is that the system is no longer described by a single eigenstate but must instead by described by a density matrix. At $t = -\infty$, the quantum impurity is decoupled from the electron bath and the system is described by the density matrix

$$\rho_0 = \exp\left(-\beta H_o\right) \qquad \beta = T^{-1}. \tag{6}$$

At later times, the system is described by time evolving the density matrix ρ_0 with the time evolution operator

$$\rho(t) = U^\dagger(t, -\infty)\, \rho_0\, U(t, -\infty) \tag{7}$$

with $U(t, -\infty)$ being understood as the limit $U(t, t_o \to -\infty)$. The expectation value of an operator $\hat{O}$ can be calculated in the usual manner by

$$\langle \hat{O} \rangle = \frac{{\rm Tr}(\rho(t)\hat{O})}{{\rm Tr}\rho(t)} \tag{8}$$

Again a time independent description can be given. Now the boundary-conditions for our evolved density matrix ρ_s is provided by ρ_0: to the left of the impurity, we know that the scattering density matrix ρ_s must reduce to ρ_0. Further, the finite temperature analogue of our zero temperature condition that our scattering state $|\Psi\rangle$ be an eigenstate of H is requirement that the density matrix ρ_s commute with the full Hamiltonian in the limit $\eta \to 0$.

Thus, at $T > 0$ we consider the incoming states, $\{|\phi, m\rangle\}$, the complete set of eigenstates of H_o with energies E_m, distributed with the probability of each state given by the Boltzman weight, $e^{-\beta E^0_m}$,

$$\rho_0 = e^{-\beta H_o} = \sum_m e^{-\beta E^0_m} |\phi, m\rangle\langle\phi, m|, \tag{9}$$

Using (7), the time-independent density matrix ρ_s is

$$\begin{aligned} \rho_s &= U(0, -\infty)\rho_o U^\dagger(0, -\infty) \\ &= \sum_m e^{-\beta E^0_m} U(0, \infty)|\phi, m\rangle\langle\phi, m| U^\dagger(0, -\infty) \\ &= \sum_m e^{-\beta E^0_m} |\Psi, m\rangle\, \langle\Psi, m| \end{aligned} \tag{10}$$

where we have used (9) and in the second line we have defined the scattering state $|\Psi, m\rangle = U(0, -\infty)|\Phi, m\rangle$ with incoming particles describe by $|\Phi, m\rangle$. The steady state physics is captured by the operator ρ_s which describes an ensemble of scattering states weighted by the Boltzman factors determined by the energy of the incoming electrons. This form for ρ_s is consistent with the requirement that ρ_s commute with the Hamiltonian and reduce to ρ_0 to the left of the impurity. We can calculate the expectation value of an operator as in (8)

$$\langle \hat{O} \rangle = \frac{{\rm Tr}(\rho_s \hat{O})}{{\rm Tr}\rho_s} \tag{11}$$

III. THE SCATTERING BETHE-ANSATZ

We have shown in the previous section that the thermodynamic properties can be obtained from scattering eigenstates defined directly on the infinite line with *incoming* boundary conditions imposed by the lead. In general, constructing such eigenstates is a formidable task

due to the strong correlations between particles, and is only carried out approximately. But for a special class of models, many of which have important direct physical application, the many-particle eigenstates can be explicitly constructed using the Bethe-Ansatz wavefunction form.

The Bethe-Ansatz approach has a long history stretching back to Bethe's study of the Heisenberg model[20]. The approach has been typically implemented on systems defined with periodic boundary conditions with respect to some finite length L. Subsequently the thermodynamic limit is achieved sending L to infinity maintaining a constant density. If a field theory limit is to be taken, then a further scaling (or universality) limit is required. By means of this "Traditional Bethe Ansatz" (TBA) approach the thermodynamics of several impurity models was studied in great detail,[17,21,22].

Scattering, on the other hand, must by definition take place in infinite systems with no boundaries - open systems in our terminology. To compute scattering properties a different formulation is required. This can be seen from several points of view. To begin with, particles must come in from asymptotic regions and after scattering occurs, escape again. Thus the system must be open to allow the flow of particles and energy in and out of the system. Furthermore, there must be a way to distinguish between the incoming particles, typically *bare* particles, eigenstates of H_o but not of H, and the renormalized quasiparticles that are the eigenstates of the latter but not of the former. Expressing the bare particles in terms of the renormalized quasiparticles and vice versa lies at the heart of the scattering theory.

Thus the traditional (or closed) Bethe-Ansatz (TBA) and the Scattering (or open) Bethe-Ansatz (SBA) naturally address different sets of questions. The natural questions that can be addressed using the first are thermodynamical. The TBA, by using a periodic system and requiring wave-functions to be self-consistent, reproduces the full renormalized excitation spectrum of a quantum-impurity model. With the knowledge of the spectrum, one can use statistical mechanics arguments to calculate the thermodynamic quantities. Boundary conditions (periodic or otherwise) imposed on a finite length system are essential to this approach. But all knowledge of the bare theory is lost. As such, the TBA is unable to tackle questions about the scattering properties of the quantum impurities. Scattering relies on working in systems with bare particles and open boundary conditions- namely systems of infinite extent with no boundaries.

There is a price to pay for working in open systems. The wavefunctions are no longer normalizable and one does not have recourse to thermodynamic concepts such as free energy. Thus, while the SBA is essential for analyzing scattering properties of quantum impurity models, it is more difficult to extract the thermodynamics using it. Table I summarizes the comparison between the two approaches.

	SBA	TBA
System	Infinite	Finite
Boundary condition	asymptotic (open)	periodic
Wavefunctions	used explicitly	not used
Thermodynamics	difficult	easy
Scattering Properties	possible	not possible
Nonequilibrium Generalization	Yes	No

TABLE I: Summary of differences between the Scattering Bethe-Ansatz (SBA) and Algebraic Bethe Ansatz (ABA).

A. The Bethe-Ansatz Wavefunction

The central objective of the SBA is to construct on the infinite line eigenstates of the Hamiltonian

$$H = H_0 + H_{\rm int} = -i\int_{-\infty}^{\infty} dx \psi_\alpha^\dagger(x)\partial_x\psi_\alpha(x) + H_{\rm int} \quad (12)$$

with the condition that far away from the quantum-impurity the incoming sector of the eigenstate reduces to a prescribed eigenstate, $|\Phi\rangle$, of the free-electron Hamiltonian H_0. As such, any scattering state must have a well-defined sense of incoming and outgoing particles, with the incoming electrons being to the left of the impurity ($x < 0$) and the outgoing scattered electrons those to its right. The state $|\Phi\rangle$ can be any eigenstate of H_0. We focus in this paper on the case where $|\Phi\rangle$ is a Fermi-sea of incoming particles. However, many other choices are possible. In particular, to calculate S-matrices and T-matrices of quantum-impurity Hamiltonian one can choose $|\Phi\rangle$ to be a Fermi-sea with one incoming particle above the Fermi-sea (see Figure 1).

The choice of $|\Phi\rangle$ describing incoming particles imposes an asymptotic boundary condition on the full scattering eigenstate. In general, imposing boundary conditions on our scattering states is quite difficult. However, when the incoming particles are a free Fermi sea, imposing the boundary-condition simplifies greatly. The key to this simplification is the observation that the natural basis for Bethe-Ansatz wavefunctions is not the Fock basis, but a new "Bethe basis" described extensively below.

The SBA constructs eigenstates of the Hamiltonian using wave-functions of Bethe-Ansatz type[20]. The Bethe-Ansatz utilizes the integrability of the Hamiltonian H to divide multi-particle scattering events into two-particle scattering events characterized by the two-particle S-matrices, S^{ij} derived from H. The integrability of the Hamiltonian translates in this language into a self-consistency condition on the two-particle S-matrices known as the Yang-Baxter Equation (YBE)[23] ensuring that all multi-particle interactions can be *consistently* broken-up into pair-wise interactions. The consistent wavefunctions of the Bethe form, which we collectively refer to as Bethe-Ansatz wavefunctions, are eigenstates of the Hamiltonian.

We restrict our analysis to quantum-impurities coupled to non-interacting electrons. We further assume that particle number is conserved, the Bethe-Ansatz wavefunctions all have a definite number of particles, N, and there are only local interactions: two particles can interact only if they are at the same point. To write a Bethe-Ansatz wavefunction, it is necessary to divide the configuration space into $N!$ regions according to the ordering of the particles on the infinite line. For example, we can consider a region where particle 5 is to the left of particle 7 which is to the left particle 9 etc., $(x_5 < x_7 < x_9 \ldots)$. Each such region is labelled by a permutation Q in the symmetric group, S_{N+1}. Since a particle i and j can only interact when they occupy the same position $x_i = x_j$, there are no interactions in the interior of these regions. Within each region, the Hamiltonian H reduces to H_0 and the eigenfunctions are sums of plane waves. The most general wave-function of the above form is (with $x_0 = 0$ the position of the impurity)

$$|BA, \{p\}\rangle = \int dx_1 \ldots dx_N \, e^{i \sum_j p_j x_j} \sum_Q A^Q_{\alpha_1 \ldots \alpha_N, \alpha_0} \theta(x_Q) \prod_{j=1}^{N} \psi^\dagger_{\alpha_j}(x_j)|0, \alpha_0\rangle \quad (13)$$

where $\theta(x_Q) = \theta(x_{Q(1)} < x_{Q(2)} \ldots x_{Q(N)} < x_{Q(0)})$ and Q runs over all $N+1!$ permutations. The state $|0, \alpha_0\rangle$ denotes the *drained* Fermi sea ($\psi_{\alpha_j}(x_j)|0\rangle = 0$) and the state of the impurity.

When a boundary between two regions is crossed, two particles interact (multi-particle interactions forbidden by Fermi statistics) and hence the amplitude in the regions across the boundary are related by a *two particle* S-matrix determined by solving the two-particle Schrodinger Equation for the relevant Hamiltonian. The amplitude in a region Q, $A_{\alpha_1 \ldots \alpha_N}(Q)$, is related to the amplitude in an adjacent region, Q', differing from it by the exchange of neighboring particles i and j, via the S-matrix S^{ij},

$$A^{Q'}_{\alpha_1 \ldots \alpha_N} = (S^{ij})^{\beta_1 \ldots \beta_N}_{\alpha_1 \ldots \alpha_N} A^Q_{\beta_1 \ldots \beta_N} = (S^{ij})^{\beta_i \beta_j}_{\alpha_i \alpha_j} A^Q_{\beta_1 \ldots \beta_N} \quad (14)$$

where in the second equality we have used the fact the two-particle S-matrix S^{ij} acts non-trivially only on the sectors of the Hilbert space corresponding to particles i and j. In general, the matrix relating the amplitude in the region $Q = I$, defined by $(x_1 < x_2 < \ldots < x_N < x_0)$ is related to the amplitude in region Q, $(x_{Q(1)} < x_{Q(2)} < \ldots < x_{Q(N)} < x_{Q(0)})$, by an S-matrix S^Q given by a product of two-particle exchange S-matrices S^{ij} along the path leading from I to Q. Since many paths can lead from I to Q consistency requires that S^Q be uniquely defined in a path independent way. This is assured by the Yang-Baxter condition[21]. Thus, the Bethe-Ansatz wavefunction can be written in terms of a single amplitude $A = A^I$ in the region $Q = I$ and the S-matrices S^Q,

$$|BA, \{p\}\rangle = \int dx_1 \ldots dx_N \, e^{\sum_j p_j x_j} \sum_Q (S^Q A)_{\alpha_1 \ldots \alpha_N} \theta(x_Q) \prod_{j=1}^{N} \psi^\dagger_{\alpha_j}(x_j)|0\rangle. \quad (15)$$

The energy of a Bethe-Ansatz wavefunction (15) is given by $E = \sum_j p_j$. Note, however, that the Bethe-Ansatz wavefunction with Bethe-Ansatz momenta, $\{p_j\}$ is degenerate in energy with all other Bethe-Ansatz wavefunctions $\{p'_j\}$ with $\sum_j p'_j = E = \sum_j p_j$. Thus, there are an infinite number of degenerate Bethe-Ansatz wavefunctions of the same energy for any Hamiltonian. Generically, a scattering state with energy E is a sum of Bethe-Ansatz wavefunctions (14)

$$|\Psi\rangle = \sum_{\{p\}; \sum_j p_j = E} C_{\{p\}} |BA, \{p\}\rangle, \quad (16)$$

with $C_{\{p\}}$ the amplitude in the scattering state of the Bethe-Ansatz wavefunction $|BA, \{p\}\rangle$ and the sum running over all sets of Bethe-Ansatz momenta $\{p\}$ with energy E.

B. The Bethe-Ansatz Basis

To construct scattering eigenstates for integrable quantum models the Bethe-Ansatz wavefunction exploits the large degeneracy of the *linearized* free electron gas. As taught in standard chapters on degenerate perturbation theory the correct basis of states in a degenerate subspace to perturb from is the one that diagonalizes the perturbation, or equivalently, the one to which the system returns once the perturbation is turned off. This is precisely the intuition behind the "Bethe basis" of a non interacting field theory. A Bethe basis for a free electron gas is the basis inherited from the interacting quantum-impurity theory when the impurity is removed, or when the system is studied far from the short range impurity. The basis is defined by the presence of a non-trivial two particle S-matrix S^{ij} between the right moving free electrons in H_0. Indeed, a moment's reflection shows that as the particles move with the same velocity (to the right with $v_F = 1$) an S-matrix does not indicate interaction but a choice of basis.

We now discuss the Bethe basis in more detail. For a quantum-impurity model, there are two kinds of two-particle S-matrices: those that describe electron-electron scattering, which we denote S^{ij}, and those that describe impurity-electron scattering which we denote S^{0j}. The S-matrices S^{ij} and S^{0j} are determined by the impurity interaction term $H_{\rm int}$ in (12) and the Yang-Baxter consistency conditions.

Imagine turning off the coupling to the impurity in (12) so that $H_{int} = 0$. Then (12) reduces to the free-field

Hamiltonian H_0 and the electron-impurity S-matrix, S^{0j} reduces to the identity, $S^{0j} \to 1$. The electron-electron S-matrix S^{ij}, however, does not change. This leads to the somewhat surprising conclusion that Bethe-Ansatz wavefunctions of the form (15) with $S^{ij} \neq 1$ are eigenstates of the free field Hamiltonian H_0.

This can be understood as follows. Consider the first quantized version of H_0. In the two-particle sector, the first quantized H_0 is given by $H_0 = -i(\partial_{x_1} + \partial_{x_2})$. Notice that any wavefunction of the form

$$|2; p_1, p_2; q\rangle = \int dx A^q_{\alpha_1\alpha_2} e^{i(p_1+q)x_1+(p_2+q)x_2} \psi^\dagger_{\alpha_1}(x_1)\psi^\dagger_{\alpha_2}(x_2)|0\rangle \quad (17)$$

is an eigenfunction of H_0 with energy $E = p_1 + p_2$ (the $\{\alpha_i\}$ label the internal degrees of freedom of the free electrons). Since q can take on any value, there is an infinite number of such states. Any sum of eigenfunctions of the above form is also an eigenfunction of the H_0 with energy E,

$$\begin{aligned} &|2; p_1, p_2\rangle = \quad (18)\\ &\sum_q \int dx_1 dx_2 e^{ip_1x_1+ip_2x_2} A^q_{\alpha_1\alpha_2} e^{iq(x_1-x_2)} \psi^\dagger_{\alpha_1}(x_1)\psi^\dagger_{\alpha_2}(x_2)|0\rangle \\ &= \int dx_1 dx_2 e^{ip_1x_1+ip_2x_2} f_{\alpha_1\alpha_2}(x_1-x_2)\psi^\dagger_{\alpha_1}(x_1)\psi^\dagger_{\alpha_2}(x_2)|0\rangle \end{aligned}$$

where to go from the first line to the second line we have used the fact that $\sum_q A^q_{\alpha_1\alpha_2} e^{iq(x_1-x_2)}$ is the general expression for the Fourier transform of an arbitrary function, $f(x_1 - x_2)$, of $x_1 - x_2$. Thus, due to the large symmetry of the free electron problem, there is an infinite number of degenerate two-particle eigenstates for H_0. The above argument easily generalizes to more than two particles: any function of the form

$$|N\rangle = \int dx_1 \dots dx_N e^{\sum_{s=1}^N p_s x_s} \prod_{i<j} f_{\alpha_i\alpha_j}(x_i - x_j) \prod_j \psi^\dagger_{\alpha_j}(x_j)|0\rangle \quad (19)$$

is an N-particle eigenstate of H_0. Since $\theta(x_Q) = \prod_{i<j}\theta(x_{Q(i)-Q(j)})$, is of that form 19 we conclude that the most general N-particle Bethe-Ansatz wavefunction with S^Q a product of electron-electron S-matrices, S^{ij},

$$|N, BA\rangle = \int d\vec{x} e^{i\sum_j p_j x_j} (S^Q A)_{\alpha_1\dots\alpha_N} \theta(x_Q) \psi^\dagger_{\alpha_1}(x_1)\dots\psi^\dagger_{\alpha_N}(x_N). \quad (20)$$

is an eigenstates of H_0. However, for $S^Q \neq 1$ (which implies $S^{ij} \neq 1$), it is clearly not of the usual Fock-basis form,

$$|N, F\rangle = \int d\vec{x} e^{i\sum_j p_j x_j} A_{\alpha_1\dots\alpha_N} \psi^\dagger_{\alpha_1}(x_1)\dots\psi^\dagger_{\alpha_N}(x_N)|0\rangle. \quad (21)$$

The different choices for S^{ij}, and in turn S^Q, correspond to different 'Bethe-Ansatz' bases for free electrons. The choice of S^{ij} imposed by the impurity interaction corresponds to working in a particular "Bethe-Ansatz" basis for the problem. The usual Fock basis corresponds to the choice $S^{ij} = 1$.

We now proceed to discuss the relationship between the Bethe basis, with $S^{ij} \neq 1$ and the Fock basis $S^{ij} = 1$. We denote, for a particular choice of a consistent set of matrices S^{ij}, the resulting Bethe-Ansatz wavefunctions by $\{|BA\rangle_n\}$ where n enumerates all possible choices for the $\{p\}$ and $A_{\alpha_1\dots\alpha_N}$ in (20). The set of Bethe-Ansatz wavefunctions $\{|BA\rangle_n\}$ form a complete basis for our Hilbert space of H_0 in the limit of infinite size and particle number. In quantum mechanics, different basis for the Hilbert space are related by unitary transformation. Thus, we can formally define an operator U that relates the Fock basis $\{|F\rangle_m\}$ to the BA basis $\{|BA\rangle_n\}$. U maps states in the Fock basis (21) to states in the Bethe-Ansatz basis (20). In general, the matrix U relating the two basis is quite complicated since a single state in the Fock basis $|F\rangle_i$ maps onto a sum of wavefunctions of the Bethe-Ansatz form $|F\rangle_n \to \sum_m U_{nm}|BA\rangle_m$. For example, in (19) we saw that the two particle eigenstate is actually a sum over many Fock states of type (17).

However, U simplifies greatly if we restrict ourselves to asking how the *ground state of* H_0 in the Bethe-Ansatz and Fock basis are related. For a systems with unique ground-states, U must map the Fock basis ground state, $|N, F\rangle_{gs}$ to the ground state in the Bethe-Ansatz basis $|N, BA\rangle_{gs}$. Thus, the ground state in the Fock basis maps to a single wavefunction of the Bethe-Ansatz form (20). Since the ground state of H_0 is a free Fermi-sea, it follows that a Fermi-sea can be represented by a single Bethe-Ansatz wavefunction. In the sections that follow, we will restrict ourselves to this case where we represent a free Fermi sea, the ground state of H_o in both basis.

C. Imposing Asymptotic Boundary-Conditions

The goal of the SBA is to construct eigenstates of the Hamiltonian (12) satisfying the asymptotic boundary-condition that the incoming particles are a prescribed eigenstate, $|\Phi\rangle$, of H_0. We focus on the simplest case when incoming particles come from a bath and are a free Fermi-sea. Central to the imposition of any boundary-condition on the fully interacting Bethe-Ansatz wavefunctions is the observation that these wave functions pick a particular Bethe-Ansatz basis for the free Hamiltonian H_0. Thus, the boundary condition, typically formulated in the Fock basis, must be reformulated in the natural basis for the scattering state wavefunctions, the Bethe-Ansatz basis. The antagonism between the Fock basis, natural for boundary-conditions, and the Bethe-Ansatz basis, natural for wavefunction is at the heart of many of the SBA. We discuss only the zero-temperature case. The generalization to finite tempera-

tures is straightforward.

Recall that the incoming electrons in our chiral picture are electrons to the left of the impurity, $x < 0$ (see Figure **??**). Thus, the asymptotic boundary condition requires that the scattering state reduce to the eigenstate of H_0, $|\Psi\rangle \to |\Phi_o\rangle = |\Phi\rangle_{baths} \otimes |\alpha_d\rangle$, when all particles are to the left of the impurity, $\{x_j\} < 0$, with $|\Phi\rangle_{bath}$ a state describing a Fermi sea of free electrons. In general, the scattering state $|\Psi\rangle$ is a sum of wavefunctions of the Bethe-Ansatz form (16). The amplitudes of the different Bethe-Ansatz wavefunctions $C_{\{p_j\}}$ are determined by the asymptotic boundary condition. It was argued in the last section that the $|\Phi\rangle_{baths}$ can be written using a *single* Bethe-Ansatz wavefunction of the form (20). Thus, in the case where the incoming particles are described by $|\Phi\rangle_{baths}$, our scattering state $|\Psi\rangle$ can also be described by a single Bethe-Ansatz wavefunction. The incoming electron corresponds to the regions in the wavefunctions of the form $\theta(x_{Q'}; x_0) \equiv \theta(x_{Q'(1)} < x_{Q'(2)} < \ldots < x_{Q'(N)} < x_0)$ with Q' a permutation of the N^e electrons in the problem. Since there are no electron-impurity scattering events in these regions, $S^{Q'}$ can be written entirely in terms of the electron-electron scattering matrix S^{ij} and the scattering state $|\Psi\rangle$ reduces to $|\Psi^-\rangle$ when all electrons are to the left of the impurity,

$$|\Psi\rangle \;\to\; |\Psi^-\rangle = \int dx_1 \ldots dx_N \, e^{i\sum_j k_j x_j} \sum_Q{}' S^{Q'} A_{\alpha_1 \ldots \alpha_{N_e}; \alpha_0} \theta(x_{Q'}; x_0) \prod_{j=1}^{N} \psi^\dagger_{\alpha_j}(x_j)|0\rangle. \tag{22}$$

The right hand side is precisely of the form (20). We therefore conclude that $|\Psi\rangle$ reduces to eigenstate of H_0 in the Bethe-Ansatz basis when all particles are to the left of the impurity. This leads to the observation that when the incoming particles are a free Fermi sea, *imposing the asymptotic boundary conditions corresponds to choosing the amplitude $A_{\alpha_1 \ldots \alpha_N}$ and the Bethe-Ansatz momenta $\{p_j\}$ for a single wavefunction of the form (20)* such that $|\Psi^-\rangle$ describes a Fermi sea.

As is usual in the Bethe-Ansatz, we do not seek to determine the BA momenta $\{p_j\}$ in the thermodynamic limit, computing, instead, the distribution function for the BA momenta, $\rho(p)$. For an infinite system, the distribution $\rho(p)$ and the amplitude $A_{\alpha_1 \ldots \alpha_N}$ are *independent* of the procedure used to arrive at them[21]. This observation allows us to find $\rho(p)$ and $A_{\alpha_1 \ldots \alpha_N}$ using an auxiliary Algebraic Bethe Ansatz problem for a system of free electrons on a finite ring of length L' with Hamiltonian H_0 and two-particle S-matrices, S^{ij}_e. In the limit $L' \to \infty$, the distribution function for the BA momenta and amplitude in the auxiliary problem will coincide with those of the physical system. $\rho(p)$ and $A_{\alpha_1 \ldots \alpha_N}$ are obtained in the auxiliary problem in the usual way by requiring that the wavefunction be periodic. In particular, the amplitude $A_{\alpha_1 \ldots \alpha_N}$ and the BA momenta $\{p_j\}$ must satisfy the auxiliary Bethe-Ansatz equations,

$$e^{ip_j L'} A_{\alpha_1 \ldots \alpha_N} = S^{jj-1} \ldots S^{j1} S^{jN} \ldots S^{jj+1} A_{\alpha_1 \ldots \alpha_N}$$

This program is carried out explicitly for the IRLM and Kondo models in the appendix.

To summarize, the imposition of the asymptotic boundary condition on the incoming particle greatly simplifies in the special case where the incoming particles are a free Fermi-sea. The scattering state $|\psi\rangle$ can be described by a single Bethe-Ansatz wavefunction and the imposition of the boundary condition is reduced to finding the amplitude and BA momenta for this BA wavefunction. These are found by using the TBA to treat the auxiliary problem of free electrons on a finite ring of length L' in the appropriate Bethe-Ansatz basis. The amplitude and the BA momenta of the auxiliary problem coincide with those of the scattering state in the limit $L' \to \infty$.

D. Computing with Scattering States

Thus far, we have discussed the explicit construction of the scattering states $|\Psi\rangle$ for integrable quantum impurity models. We proceed now to compute the expectation values of physical quantities in the scattering eigenstates using (4)

$$\langle \hat{O} \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \tag{23}$$

The calculations of expectation values are greatly simplified because we work directly with infinite systems. Technically, this is because for strictly infinite systems, we can ignore all but one term in the Slater-determinants occurring in the above expression. This simplification is the mathematical expression of the physics for infinite systems: electrons that scatter off the impurity "leave" the system and never return to scatter off the impurity again.

Consider first the overlap between two Bethe-Ansatz wavefunctions. Since they are given as a sum of plane waves in each region Q, the overlap of two such-wavefunctions, $\langle BA, \{p_j\} | BA, \{k_j\} \rangle$, is (suppressing the internal index α_j for notational brevity)

$$\sum_{Q,\tilde{Q}} \int d\vec{x} d\vec{y} \, e^{i\sum_j (k_j x_j - p_j y_j)} \theta(x_Q)\theta(y_{\tilde{Q}}) \; A(Q)A(\tilde{Q}) \langle 0| \prod_{s=1}^{N} \psi(y_s) \prod_{j=1}^{N} \psi^\dagger(x_j)|0\rangle \tag{24}$$

The Fermions field give rise to a Slater determinant

$$\sum_{Q,\tilde{Q},S} (-1)^{sgn(S)} \int d\vec{x} d\vec{y} \, e^{i\sum_j (k_j x_j - p_j y_j)} \theta(x_Q)\theta(y_{\tilde{Q}}) \; A(Q)A(\tilde{Q}) \prod_{j=1}^{N} \delta(x_{S(j)} - y_j) \tag{25}$$

where S is a permutation of the N particles. Integrating over $\vec{y}$, we have

$$\langle BA,\{p_j\}|BA,\{k_j\}\rangle = \tag{26}$$
$$=\sum_{Q,S}(-1)^{sgn(S)}\int d\vec{x}\, e^{i\sum_j(k_j x_j - p_j x_{S(j)})}\theta(x_Q)A(Q)A(QS^{-1})$$
$$=\sum_{Q,S}(-1)^{sgn(S)}\int d\vec{x}\, e^{i\sum_j(k_j - p_{S^{-1}(j)})x_j}\theta(x_Q)A(Q)A(QS^{-1})$$

Thus, we see that this expression is the norm of plane waves integrated over a region $\theta(x_Q)$. As is usual we regularize plane waves by first placing the system in a box of size L whose size is then taken to infinity at the end of the calculation. This allows us to consider the simpler problem of plane-waves

$$\lim_{L\to\infty}\int_{-L/2}^{L/2} dx e^{i(k_j-p_j)x_j}\theta(x_1 < x_2 \ldots < x_N). \tag{27}$$

It is straightforward to show that the leading order contribution in L to this integral is $L^N/N!$ which occurs only if the two sets of Bethe-Ansatz momenta are identical $\{k_j\} = \{p_j\}$. This is the statement that plane waves are 'orthogonal' even on a region $\theta(x_Q)$ for an infinite system. Thus, for infinite size systems we can ignore all terms in (26) where the $k_j \neq p_{S^{-1}(j)}$ for all j.. This leads to great technical simplifications as we only need to keep terms in the sum (26) where $Q = 1$. Similar, simplifications occur when computing the expectation value of an operator $\hat{O}$ between Bethe-Ansatz wavefunctions.

IV. SCATTERING APPROACH TO THE RESONANT LEVEL MODEL

In this section, we will apply the scattering framework to a quadratic model, the Resonance Level Model (RLM). Despite its simplicity there is much interest in this model because it describes the strong coupling physics of the Kondo model. It will be shown that our results agree with other approaches to this model such as Keldysh or Landauer which can be carried out completely in this quadratic case. In the next section we shall apply our approach to a fully interacting model with strong correlations.

The Hamiltonian for the RLM,

$$\begin{aligned} H_{\rm RL} &= H_0 + H_{RL\rm int} \qquad (28)\\ H_0 &= -i\int dx\,\psi^\dagger(x)\partial_x\psi(x)\\ H_{RL\rm int} &= t(\psi^\dagger(0)d + h.c.) + \epsilon_d d^\dagger d, \end{aligned}$$

describes a local level $d^\dagger$ onto which electrons can hop on and off. The energy of the level (relative to the Fermi energy) is controlled by ϵ_d, related to the magnetic field in the anisotropic Kondo[24]. Notice, that we have already projected to one dimension and there are only right moving chiral electrons. As explained in the last sections, in the chiral picture, the free incoming electrons are located to the left of the impurity, $x < 0$, and the scattered outgoing electrons are to the right of the impurity, $x > 0$. The RLM serves as a good pedagogical introduction to the scattering framework for quantum impurity models since it is quadratic model and we will not have to resort to the full machinery of the scattering Bethe-Ansatz.

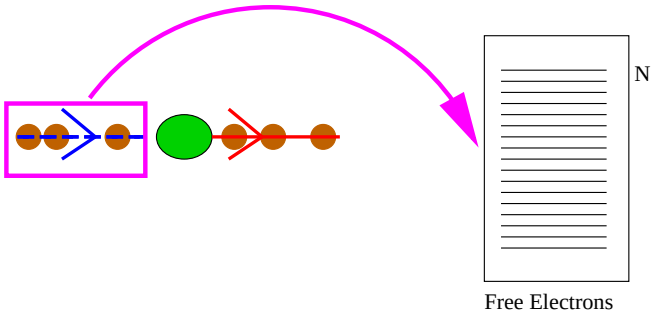

FIG. 2: The scattering state $|\psi\rangle$ describes a quantum-impurity where the incoming particles ($\{x_i < 0\}$) are a free Fermi-sea with N particles.

A. RLM at $T = 0$: Thermodynamical Properties

Consider first the zero temperature thermodynamics. We must construct a 'in' scattering state, $|\Psi\rangle_s$, describing incoming electrons from the host metal scattering off the impurity. The scattering state $|\Psi\rangle_s$ is an eigenstate of the full Hamiltonian (28) such that when all the particles are to the left of the impurity $|\Psi\rangle_s$ reduces to an eigenstate $|\Phi_o\rangle$ of H_0 describing a Fermi see (see Figure2).

The RLM Hamiltonian (28) conserves total particle number. Hence, we can work in a sector of the Hilbert space with a definite number of particles, N. Beginning with $N = 1$, the most general single particle eigenstate is of the form

$$|1p\rangle_s = \left(\int_{-\infty}^{\infty} dx e^{ipx} g_p(x)\psi^\dagger(x) + e_p d^\dagger\right)|0\rangle \tag{29}$$

Applying the Hamiltonian leads to Schrodinger equation

$$\begin{aligned} \partial_x g_p(x) + V e_p\delta(x) &= p g_p(x) \qquad (30)\\ t g_p(0) + \epsilon_d e_p &= p e_p. \qquad (31) \end{aligned}$$

Taking the ansatz that $g_p(x)$ is of the form $g_p(x) = A\theta(-x) + B\theta(x)$ and inserting this into the above equation, one has, using the regularization scheme $\delta(x)\theta(x) = \frac{1}{2}\delta(x)$[21], that

$$\frac{B}{A} = \frac{1 + i\frac{t^2}{2(p-\epsilon_d)}}{1 - i\frac{t^2}{2(p-\epsilon_d)}} \equiv e^{i\delta_p} \tag{32}$$

Thus, the most general single particle eigenstate is given

by

$$|1p\rangle_s = \left(\int dx e^{ipx} A(\theta(-x) + e^{i\delta_p}\theta(x)) + e_p d^\dagger\right)|0\rangle$$
$$e_p = \frac{tg(0)}{(p-\epsilon_d)} = \frac{t(1+e^{i\delta_p})}{2(p-\epsilon_d)} \quad (33)$$

where to get the second equation we have used (31) and the aforementioned regularization scheme. For future reference it will be helpful to define the single particle scattering state creation operator

$$\alpha_p^\dagger(x) = (\theta(-x) + e^{i\delta_p}\theta(x))\psi^\dagger(x) + \delta(x)e_p d^\dagger \quad (34)$$

Since the Hamiltonian (28) is quadratic, a N-particle eigenstate is given by a tensor product of single particle eigenstates. The most general N-particle eigenstate is of the form

$$|\Psi\rangle = \prod_{j=1}^N \otimes |1p_j\rangle = \prod_{j=1}^N \int d\vec{x} e^{i\sum_j p_j x_j} \alpha_{p_j}^\dagger(x_j)|0\rangle \quad (35)$$

Notice that we have not yet specified the momenta $\{p_j\}$ of the state. Since we wish to construct a scattering eigenstate, these momenta must be chosen to satisfy the boundary condition that when all particles are to the left of the impurity our eigenstate reduces to an eigenstate of H_o describing the incoming electrons of the host metal or lead at thermal equilibrium (see Figure 2). At zero temperature, this means that the scattering state must reduce to $|\Phi_o\rangle = |\Phi\rangle_{baths} \otimes |\phi_d\rangle$, when all particles are to the left of the impurity. Here $|\phi_d\rangle$ describes some impurity state and $|\Phi\rangle_{baths}$ describes a free Fermi sea

$$|\Phi\rangle_{baths} = \int dx_1 \dots dx_N e^{i\sum_{j=1}^N p_j x_j} \psi^\dagger(x_1)\dots\psi^\dagger(x_N)|0\rangle \quad (36)$$

under the *additional condition* that the momenta of the particles $\{p_j\}$ be distributed according to the Fermi-Dirac distribution function. Since we are interested in the limit where the number of particles goes to infinity, it is sufficient to specify the distribution of the momenta instead of the individual values of the momenta themselves.

The single particle eigenstate (33) consists of an incoming particle, $\int dx\theta(-x)e^{ipx}\psi^\dagger(x)|0\rangle$, and an outgoing scattered wave, $\int dx\theta(x)e^{i(px+\delta_p)}\psi^\dagger(x)|0\rangle$. Since the multi-particle scattering state (35) is a tensor product of the single particle state, when all particles are to the left of the impurity $|\psi\rangle_s$ reduces to

$$|\Psi\rangle_s \to \quad (37)$$
$$\int dx_1 \dots dx_N \prod_{s=1}^N \theta(-x_s) e^{i\sum_{j=1}^N p_j x_j} \psi^\dagger(x_1)\dots\psi^\dagger(x_N)|0\rangle.$$

If we choose the momenta $\{p_j\}$ to be distributed according to the Fermi-Dirac distribution, (35) reduces to the expression for $|\Phi\rangle_{baths}$. Hence, our scattering state is given by (35) with the requirement that the momentum distribution of the electrons be chosen according to the Fermi-Dirac distribution.

Expectation values We can calculate the expectation value of operators for the RL model using (4). We are interested in calculating the dot occupation $n_d = \langle d^\dagger d\rangle$. Since the multi-particle eigenstate (35) is a tensor product of single particle eigenstates (33), it is useful to prove some identities about single-particle scattering states. We regularize our system, as is usual in scattering theory, by placing the system in a box of length L. The physical system corresponds only to the $L = \infty$ limit and finite L properties are *not* well defined. A straightforward calculations yields (without loss of generality setting $A = 1$ in (33))

$$\langle 1k|1p\rangle = \quad (38)$$
$$L\delta_{pk} + \left[|e^p|^2\delta_{pk} + \left(\frac{1-e^{i(\delta_p-\delta_k)L}}{i(p-k)}\right)(1-\delta_{pk})\right]$$

and

$$\langle 1k|d^\dagger d|1p\rangle = e_k^* e_p \quad (39)$$

Thus the overlap of states with the same momenta is of higher order in L than those with different momenta, so that plane waves are an orthogonal basis for infinite size systems. In the scattering framework which works directly with infinite size systems, it is sufficient to consider overlaps only of single-particle states with the same momenta.

Consider now the dot occupation. To leading order in L, one finds, combining (39), (38), (35), and (4), that the occupation is given by

$$\langle n_d\rangle = \frac{1}{L}\sum_{j=1}^N \frac{|e_{p_j}|^2}{|1+e^{i\delta_{p_j}}|^2} = \frac{1}{L}\sum_{j=1}^{N_1} \frac{2\Delta}{\Delta^2 + (p_j-\epsilon_d)^2} \quad (40)$$

with $\Delta = t^2/2$, where to go from the first to the second line we have used the explicit forms of e_p and $e^{i\delta_p}$. Since, we are interested in the infinite size limit $N, L \to \infty$, we can replace the sum by an integral over the distribution of incoming electrons which is given by the Fermi-Dirac distribution function, $\theta(\epsilon_f - p)$ to yield

$$\langle n_d\rangle = \int dp\,\theta(\epsilon_f - p)\frac{2\Delta}{(p_j-\epsilon_d)^2 + \Delta^2} \quad (41)$$

.

We compare this result to the one from the traditional Bethe-Ansatz, defined with periodic boundary conditions on a ring of length L. In the usual Bethe-Ansatz, one puts the system on a circle and imposes the self consistency condition that $|\psi\rangle$ at $x = 0$ equals $|\psi\rangle$ at $x_j = L$[21]. This leads to the B.A. equations. For this model where the two-particle S-matrices are trivial, the B.A. equations yield for the energy

$$E = \sum p_j = \sum_j \left(\frac{2\pi n_j}{L} + \frac{1}{L}\delta_{p_j}\right). \quad (42)$$

The $\{n_j\}$ are integers corresponding to the energy of a free electron and the $\{\delta_{p_j}\}$ the shift in the energies due to the impurity. For future reference, define the 'impurity' energy as $E_{imp} = \lim_{L\to\infty} \frac{1}{L}\sum_j \delta_{p_j} = \int dp\rho(p)\delta(p)$ with $\rho(p)$ the distribution that describes the free electrons in the Bethe-Ansatz basis. From the Feynman Hellman theorem[18], we know that

$$\begin{aligned}\langle n_d\rangle &= \frac{\partial E}{\partial \epsilon_d} = \frac{\partial E_{imp}}{\partial \epsilon_d} = \frac{1}{L}\sum_j \frac{2\Delta}{(p_j-\epsilon_d)^2+\Delta^2} \\ &= \int dp\,\theta(E_f-p)\frac{2\Delta}{(p_j-\epsilon_d)^2+\Delta^2} \end{aligned} \tag{43}$$

in agreement with the expression we computed using the scattering state formalism (41).

It is helpful to define an operator that directly yields the impurity energy using scattering states. This is done by considering the overlap of the outgoing scattered waves with the unscattered Fermi-sea. Define a state $|\Phi^+\rangle$ that describes a bath of outgoing particles (i.e. all particles are to the right of the impurity)

$$|\Phi_o^+\rangle = \int \prod_i^n dx_i \prod_{s=1}^N \theta(x_s) e^{i\sum_{j=1}^N p_j x_j}\psi^\dagger(x_1)\dots\psi^\dagger(x_N)|0\rangle$$

Then, we can define impurity energy alternatively in terms of an impurity energy operator, $\hat{E}_{imp}$, that acts on scattering state $|\psi\rangle$

$$\hat{E}_{imp}|\Psi\rangle = \lim_{L\to\infty}\frac{-i}{L}\log\left(\frac{\langle\Phi^+|\Psi\rangle}{\langle\Phi^+|\Phi^+\rangle}\right)|\Psi\rangle.$$

A straightforward calculation shows that the expectation value of impurity-energy operator

$$\langle\hat{E}_{imp}\rangle = \lim_{L\to\infty}\frac{\langle\Psi|\hat{E}_{imp}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{1}{L}\sum_j \delta_{p_j} = \int dp\rho(p)\delta(p) \tag{44}$$

agrees with the expression derived from traditional methods. The virtue of this operator is that it can be generalized in a straightforward manner to all integrable quantum-impurity models. This object is closely related to the many-body T-matrix for the quantum-impurity model.

RLM at Finite Temperatures: Thermodynamical Properties Consider now the finite temperature case. At finite temperature, $T > 0$, the system is no longer described by single scattering eigenstate. Instead, we must consider a density matrix of the form (10) composed of scattering states weighted by the thermal Boltzmann distribution. Label the set of N-particle scattering states by the energy of the incoming electrons $\{|\psi, m\rangle\}$, with m labelling all possible sets of energies for the particles $p_1 < p_2 < \ldots < p_N$. We expect that these scattering states are a complete basis for the Hilbert space, and indeed find that this assumption reproduces known thermodynamic results correctly.

We calculate the finite temperature properties of the RLM using (11). The dot expectation value is calculated using dot occupation operator $\hat{n}_d = d^\dagger d$:

$$\begin{aligned}\langle\hat{n}_d\rangle &= \frac{\mathrm{Tr}(\rho_s\hat{n}_d)}{\mathrm{Tr}\rho_s} = \frac{\mathrm{Tr}\sum_m e^{-\beta E_m^0}|\psi,m\rangle\langle\psi,m|\hat{n}_d}{\mathrm{Tr}\sum_m e^{-\beta E_m^0}|\psi,m\rangle\langle\psi,m|} \\ &= \frac{\sum_{m,n} e^{-\beta E_m^0}\langle\psi,n|\psi,m\rangle\langle\psi,m|\hat{n}_d|\psi,n\rangle}{\sum_{m',n} e^{-\beta E_{m'}^0}|\langle\psi,n|\psi,m'\rangle|^2}\end{aligned}$$

The above expressions simplify when we work in the infinite physical L limit since we can keep only leading order terms in L. Recall, that m, m' and n are shorthand labels for the ordered set of energies of the N electrons $p_1 < p_2 < \ldots < p_N$. Thus, if $m \neq n$, there is at least one electron in each state with different energy. Furthermore,notice that the overlaps of a single particle eigenstates (33) given by (38) are leading order in L only if the energies of the two single particle eigenstates coincide. Hence, we conclude from (35) that the leading order in L contribution to the overlap of multi-particle eigenstates comes from states where *all* particles have the same energy, or in other words, when the two states are identical. Thus, for the infinite L limit, we can set $m = m' = n$ in the above expressions to get

$$\begin{aligned}\langle\hat{n}_d\rangle &= \sum_n \frac{e^{-\beta E_n^0}}{\sum_{m'} e^{-\beta E_{m'}^0}}\frac{\langle\psi,n|\hat{n}_d|\psi,n\rangle}{L^N} \\ &\equiv \sum_n P(n)\frac{\langle\psi,n|\hat{n}_d|\psi,n\rangle}{L^N} \\ &= \sum_n \frac{P(n)}{L}\sum_{p_j\in\{p_j\}_n}\frac{2\Delta}{\Delta^2+(p_j-\epsilon_d)^2} \\ &\equiv \sum_n \frac{P(n)}{L}\sum_{p_j\in\{p_j\}_n} n_d(\epsilon)\end{aligned} \tag{45}$$

where $P(n)$ is the Boltzman probability for the state labelled by n. We can now use a standard trick of statistical mechanics and replace the sum over all configurations by an integral over the average occupancy of a level of energy p, $N(p)$, which in this case is given by the finite-temperature Fermi-Dirac distribution function, $f(p,T)$. This yields

$$\langle\hat{n}_d\rangle = \int dp\, f(p,T)\frac{2\Delta}{(p_j-\epsilon_d)^2+\Delta^2}. \tag{46}$$

Thus, the effect of temperature is then incorporated by requiring that the momentum distribution of the incoming electrons be chosen according to the finite temperature Fermi-Dirac distribution for free electrons. This expression is in agreement with known results. We will see that the above argument is quite general and that the effect of temperature can be generically incorporated by integrating over finite-temperature distribution functions instead of their zero-temperature counterparts.

An almost analogous calculation using the impurity energy operator $\hat{E}_{imp}$ yields that the finite energy impurity

energy is

$$\langle \hat{E}_{imp} \rangle = \int dp\, f(p,T)\delta_p. \tag{47}$$

The great limitation of the scattering formalism is that though we can calculate the finite temperature energy, calculating the free energy is much trickier. A free energy operator can also be defined for these models though this is much trickier and will not be discussed in this paper[25].

V. SCATTERING APPROACH TO THE INTERACTING RESONANCE MODEL (IRLM) THERMODYNAMICS

In this section, we compute the zero temperature thermodynamic properties of the interacting Resonance Level Model (IRLM) within the scattering framework. The IRLM Hamiltonian,

$$\begin{aligned} H_{\rm IRLM} &= H_0 + H_I = -i\int dx \psi^\dagger(x)\partial_x\psi(x) + H_I \\ &= -i\int dx\, \psi^\dagger(x)\partial_x\psi(x) + t(\psi^\dagger(0)d + h.c.) \\ &\quad + U\,\psi^\dagger(0)\psi(0)d^\dagger d + \epsilon_d d^\dagger d \end{aligned}$$

describes a local level, $d^\dagger$, onto which spinless electrons hop on and off. There is an additional Coulomb interaction between the level and electrons. We consider only the case where $\epsilon_d > 0$, where the level is above the Fermi energy of the electrons. Unlike the RLM considered earlier, this model is no longer quadratic and we must use the full Scattering Bethe-Ansatz (SBA) technology to construct scattering states.

We construct the scattering states. They satisfy the Lippman-Schwinger equation (5), and specifying the boundary condition on the incoming particles, $|\Phi\rangle$, and the Hamiltonian (48), uniquely determine the corresponding scattering state $|\Psi\rangle$. In this section, we restrict ourselves to scattering states where the incoming particles are a Fermi-sea at zero temperature $|\Phi_o\rangle$. Such scattering states are sufficient to describe the zero temperature thermodynamic properties of the IRLM such as the dot occupation and impurity energy.

In principle, the scattering formalism can also be used to describe quasi-particle S and T matrices. We defer these topics to future publications as they require treating more complicated boundary condition for incoming particles that includes quasi-particle excitations above the Fermi-sea.

A. Construction of the scattering state

The scattering states for the IRLM are constructed using the SBA, directly in open systems of infinite size, $L \to \infty$. The most general N-particle eigenstate is of the Bethe-Ansatz form

$$|\{p\}\rangle = A\int d\vec{x} e^{\frac{i}{2}\sum_{i<j} sgn(x_i - x_j)\Phi(p_i,p_j)} \prod_{j=1}^{N} \alpha^\dagger_{p_j}(x_j)|0\rangle \tag{48}$$

with

$$\Phi(p.k) = \tan^{-1}\left(\frac{U(p-k)}{2(p+k-2\epsilon_d)}\right) \tag{49}$$

and δ_p and e_p given in (32) and (33)[26]. Note that $\alpha^\dagger$ is the operator that creates a single-particle eigenstate (34) in the non-interacting RLM. The states $|\{p\}\rangle$ are a complete set of states in terms of which a particular scattering state can be constructed as a linear combination of by the set ($\{p\}$) determined by the boundary conditions. In our case the boundary condition requires that the incoming particles look like a free Fermi sea. As discussed previously, for this boundary condition a single state $|\{p\}\rangle$ with appropriately chosen set $\{p\}$ suffices to determine $|\Psi\rangle_s$. In more detail, when all the particles are to the left on the impurity, $\{x_i\} < 0$, $|\Psi\rangle_s$ must reduce to an eigenstate of H_0, $|\Phi_o\rangle$, describing a zero temperature Fermi sea and a decoupled impurity. When all the $\{x_j\} < 0$, the operators $\{\alpha^\dagger_{p_j}(x_j)\}$ reduce to $\{e^{ip_j x_j}\psi^\dagger(x_j)\}$ and the eigenstate $|\Psi\rangle_s$ reduces to

$$|\psi\rangle \to \int d\vec{x} A e^{\frac{i}{2}\sum_{i<j} sgn(x_i-x_j)\Phi(p_i,p_j)} e^{i\sum_j x_j p_j} \prod_{j=1}^{N}\psi^\dagger(x_j)|0\rangle.$$

Thus, we must choose the $\{p_j\}$ in such a manner that the above expression describes a free Fermi sea.

Despite its appearance the expression on the right hand side is an eigenstate of H_o. This can be seen by applying $h_o = -i\sum_{j=1}^{N}\partial_{x_j}$ to the wave function. Indeed, since all particles are right mover the scattering S-matric $S = e^{i\Phi(p_i,p_j)}$ describes the choice of a Bethe basis in the infinitely degenerate energy subspace of free electrons. Thus, for $\{x_j\} < 0$, $|\Psi\rangle_s$ reduces to an eigenstate expressed in the Bethe basis characterized by the two-particle S-matrix $S = e^{i\Phi(p_i,p_j)}$. This Bethe basis is the natural basis for our problem since, as discussed previously, degenerate perturbation theory demands that we choose the basis for the free electron eigenstates by "turning off" the perturbation, in this case the coupling to the quantum impurity. It is worth emphasizing that the momenta $\{p_j\}$ should coincide with the usual Fock momenta of quasi-particles only when $U = 0$ and the $S^{ij} = 1$.

The boundary-condition on incoming particles must be implemented in the Bethe-Ansatz basis with a non-trivial two particle electron S-matrix $S = e^{i\Phi(p_i,p_j)}$. As discussed previously, the requirement that the incoming particles be a Fermi sea translates in this Bethe basis into the condition that in $|\Phi_o\rangle$ the incoming particles be an

eigenstate of H_0 of the form (20)

$$|\Phi\rangle_{bath} = A\int d\vec{x} e^{i\sum_j p_j x_j} e^{\frac{i}{2}\sum_{i<j} sgn(x_i-x_j)\Phi(p_i,p_j)} \psi^\dagger(x_1)\dots\psi^\dagger(x_N)|0\rangle \quad (50)$$

with the additional condition that the distribution for the BA momenta of the incoming particles, $\rho(p)$, satisfy a set of free Bethe-Ansatz equations for an *auxiliary* problem of free electrons on a ring of length L' with a two particle S-matrix, $S = \exp(i\Phi(p,k))$. These equations are derived in the appendix (A9) and are given by,

$$\begin{aligned} \rho(p) &= \frac{1}{2\pi} - \int dk \rho(k) K(p,k) \quad (51)\\ K(p,k) &= \frac{1}{2\pi}\frac{\partial\Phi(p,k)}{\partial p} = \frac{U}{\pi}\frac{(\epsilon_d - k)}{(p+k-2\epsilon_d)^2 + \frac{U^2}{4}(p-k)^2}. \end{aligned}$$

The desired scattering state, $|\Psi\rangle_s$, is given by (48) with *the additional requirement* that the distribution of the BA momenta, $\rho(p)$, solves the Bethe-Ansatz equation above. The simplicity of the equation follows from the fact the ground states in the Fock basis and in the Bethe basis are unique. This is no longer the case for excited excited states. It is also worth emphasizing that (52) correspond to a free Hamiltonian H_0 and thus differ from the usual Bethe-Ansatz equations for the IRLM[26] in that they contain no impurity contribution.

B. Zero Temperature Properties

Having constructed scattering states, we now use them to calculate the thermodynamic properties of the IRLM. In particular, we will use scattering states to calculate the zero-temperature dot occupation $\langle\hat{n}_d\rangle = \langle d^\dagger d\rangle$ and the impurity energy E_{imp} defined as using the impurity energy operator (44). At zero temperature, E_{imp} plays the role of the free-energy for all dot thermodynamic properties. We then show that our results agree with those derived using traditional Bethe-Ansatz techniques.

To calculate the impurity dot occupation we use (4) which yields

$$\langle\hat{n}_d\rangle = \frac{\langle\Psi|d^\dagger d|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \quad (52)$$

with $|\Psi\rangle$ as in (48). As is usual in scattering theory, we regularize our calculations by placing the system in a box of size L. Since scattering is defined only for open systems, the physical system correspond to the infinite L limit and finite L properties are *not* well defined. From the definition of $\alpha^\dagger$ (34), it follows that $d^\dagger d\alpha^\dagger_{p_s}(x_s)|0\rangle = \delta(x_s)e_{p_s}d^\dagger|0\rangle$. Thus,

$$\begin{aligned} \langle\Psi|d^\dagger d|\Psi\rangle = \sum(-1)^s A^2 \int d\vec{y}\, d\vec{x}\, \delta(x_s) \\ \times\ e^{\frac{i}{2}\sum_{i<j}(sgn(x_i-x_j)-sgn(y_i-y_j))\Phi(p_i,p_j)} \\ \times\ e_{p_s}\prod_{j',j=1,j\neq s}^{N}\langle 0|\alpha_{j'}(y_{j'})d^\dagger\alpha_j^\dagger(x_j)|0\rangle \quad (53) \end{aligned}$$

A very similar calculation yields

$$\begin{aligned} \langle\Psi|\Psi\rangle =& A^2\int d\vec{y}\, d\vec{x}\, e^{\frac{i}{2}\sum_{i<j}(sgn(x_i-x_j)-sgn(y_i-y_j))\Phi(p_i,p_j)} \\ & \prod_{j',j=1}^{N}\langle 0|\alpha_{j'}(y_{j'})\alpha_j^\dagger(x_j)|0\rangle \quad (54) \end{aligned}$$

To proceed with the calculation we note that from (34), one has the relations

$$\begin{aligned} \{\alpha_j(x_j),\alpha_s^\dagger(x_s)\} &= e^{i(p_s-p_j)}[\theta(-x_s)+e^{i(\delta_{p_s}-\delta_{p_j})}\theta(x_s)] \\ &\quad\times\delta(x_s-x_j) + e_{p_j}e_{p_s}\delta(x_s)\delta(x_j) \\ \{d,\alpha_s^\dagger(x_s)\} &= e_{p_s}\delta(x_s) \quad (55) \end{aligned}$$

The right hand side of the first equation has two terms: the first term proportional to $\delta(x_s-x_j)$ comes from the anti-commutation of the fermionic field ψ while the second comes from d. When calculating (53) and (54) keeping only the first term is sufficient to get the leading order in L in the dot occupation since the first term contains only one delta function where as the second contains two. In explicitly open systems where L in infinite, it is sufficient to treat the anti-commutation relation as

$$\begin{aligned} \{\alpha_j(x_j),\alpha_s^\dagger(x_s)\} \approx e^{i(p_s-p_j)} \quad (56)\\ \times[\theta(-x_s)e^{i(\delta_{p_s}-\delta_{p_j})}\theta(x_s)]\delta(x_s-x_j) \end{aligned}$$

Then, the norm to leading order in L is given by

$$\begin{aligned} &\langle\Psi|\Psi\rangle = A^2\sum_{\sigma\in S_N}(-1)^{sgn\sigma} \\ &\int d\vec{y}\, d\vec{x}\, e^{\frac{i}{2}\sum_{i<j}(sgn(x_i-x_j)(\Phi(p_i,p_j)-\Phi(p_{\sigma(i)},p_{\sigma(j)}))} \\ &\prod_{s=1}^{N} e^{i(p_s-p_{\sigma(s)})x_s}[\theta(-x_s)+e^{i(\delta_{p_s}-\delta_{p_{\sigma(s)}})}\theta(x_s)]\delta(y_{\sigma(s)}-x_s) \end{aligned}$$

The integral over y is trivial. As explained in the last section, the leading order in L contribution to such an integral comes when $e^{i(p_s-p_{\sigma(s)})x_s}=1$ or precisely when the permutation $\sigma=1$. In this case the integral is performed trivially and yields $\langle\Psi|\Psi\rangle = A^2L^N$. An analogous calculation using (53) yields to leading order in L that $\langle\Psi|d^\dagger d|\Psi\rangle = A^2L^{N-1}\sum_{j=1}^N|e_{p_s}|^2$. Combining these two results yields

$$\langle\hat{n}_d\rangle = \frac{\langle\Psi|d^\dagger d|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{1}{L}\sum_{s=1}^{N}|e_{p_s}|^2 = \frac{1}{L}\sum_{s=1}^{N}\frac{2\Delta}{\Delta^2+(p-\epsilon_d)^2}$$

where we have defined the hybridization $\Delta = t^2/2$. In the, infinite L, infinite N limit, we can replace the sum by an integral over the distribution of BA momenta for the incoming particles, $\rho(p)$ given by (A9) to get

$$\langle \hat{n}_d \rangle = \int dp\, \rho(p) \frac{2\Delta}{\Delta^2 + (p-\epsilon_d)^2} \tag{57}$$

We can also compute the impurity-energy using the impurity energy operator

$$E_{imp} = \frac{-i}{L} \log\left(\frac{\langle \Phi^+ | \Psi \rangle}{\langle \Phi^+ | \Phi^+ \rangle} \right) \tag{58}$$

where $|\Phi^+\rangle$ is the eigenstate of the free bath given by (59) with the additional requirement that all particles be to the right of the impurity:

$$\begin{aligned} |\Phi^+\rangle &= A \int d\vec{x} \prod_{s=1}^{N} \theta(x_s) e^{i\sum_j p_j x_j} e^{\frac{i}{2}\sum_{i<j} sgn(x_i - x_j)\Phi(p_i,p_j)} \\ &\quad \psi^\dagger(x_1) \dots \psi^\dagger(x_N)|0\rangle. \end{aligned} \tag{59}$$

These correspond to outgoing free Fermi-sea of scattered electrons. In this case,

$$\begin{aligned} \langle \Phi^+ | \psi \rangle &= \int d\vec{y}\, d\vec{x}\, e^{\frac{i}{2}\sum_{i<j}(sgn(x_i-x_j) - sgn(y_i - y_j))\Phi(p_i,p_j)} \\ &\quad \times \prod_{j',j=1}^{N} e^{-ip_{j'} y_{j'}} \theta(y_{j'}) \langle 0|\psi(y_{j'}) \alpha_j^\dagger(x_j)|0\rangle \\ &= A^2 \sum_{\sigma \in S_N} (-1)^{sgn\sigma} \int d\vec{y}\, d\vec{x} \\ &\quad e^{\frac{i}{2}\sum_{i<j}(sgn(x_i-x_j)(\Phi(p_i,p_j) - \Phi(p_{\sigma(i)},p_{\sigma(j)}))} \\ &\quad \times \prod_{s=1}^{N} e^{i(p_s - p_{\sigma(s)})x_s} e^{i\delta_{p_s}} \theta(x_s) \delta(y_{\sigma(s)} - x_s) \end{aligned} \tag{60}$$

Once again the integral over y is trivial and the leading order in L contribution comes from when the permutation $\sigma = 1$ This yields $\langle \Phi^+ | \psi \rangle = A^2 (L/2)^N e^{i\sum_{s=1}^{N} \delta_{p_s}}$. An almost identical calculation to the one used to calculate $\langle \psi | \psi \rangle$ gives $\langle \Phi^+ | \Phi^+ \rangle = A^2 (L/2)^N$. Combining these results and substituting in (58) gives

$$\langle \hat{E}_{imp} \rangle = \frac{-i}{L} \log\left(\frac{\langle \Phi^+ | \psi \rangle}{\langle \Phi^+ | \Phi^+ \rangle} \right) = \frac{1}{L} \sum_{s=1}^{N} \delta_{p_s} \tag{61}$$

We can once again replace the sum by integrals over $\rho(p)$ to get

$$E_{imp} = \int dp\ \rho(p) \delta_p. \tag{62}$$

These results can be checked with those arrived at using the traditional Bethe-Ansatz (TBA)[26]. The TBA results are almost identical to those from the SBA except that the distribution $\rho(p)$ must be replaced by TBA distributions $\rho_I(p)$ that include a contribution from the impurity,

$$\begin{aligned} E_{imp} &= \int dp\ \rho_I(p) \delta_p \\ \langle \hat{n}_d \rangle &= \int dp\, \rho_I(p) \frac{2\Delta}{\Delta^2 + (p-\epsilon_d)^2} \end{aligned} \tag{63}$$

Since, as pointed out in[26], the distributions for the TBA, $\rho_I(p)$, differs from the distribution from the SBA, $\rho(p)$, by a term proportional to N^{-1} where N is the number of particles, in the $L, N \to \infty$ limit, the SBA and TBA expressions coincide.

VI. SCATTERING APPROACH TO THE KONDO THERMODYNAMICS

In this section, we discuss how the scattering Bethe-Ansatz could be used to calculate interesting physical quantities in the Kondo model. Due to the complexity of the scattering state for the Kondo model, doing concrete calculations requires the generalization of many mathematical methods described in the context of spin chains. In particular, we discuss the tantalizing possibility that many of the methods of Maillet, Terras, and collaborators[27] can be generalized to the Kondo model where they may allow exact calculation of as yet inaccessible interesting physical quantities such as the impurity T-matrix. The section starts with a brief discussion of the scattering state that captures the thermodynamics of the Kondo problem. In the next subsection, we discuss a possible mapping between the Kondo problem and an auxiliary 'abelian' problem similar to the IRLM model. Finally, we discuss how to calculate quantities in this auxiliary problem and discuss how this formalism may be generalized. We concentrate only on the zero temperature properties of the Kondo model. The generalization to finite temperatures will be presented later.

A. The Scattering State

The scattering state for the Kondo model is significantly more complicated than that for the IRLM. These extra complications stem from the non-abelian nature of the electron two-particle S-matrices in the Kondo model, $S_e^{ij} = P^{ij}$. This is already evident in the appendix where we represent the free-Fermi seas in the Kondo Bethe-Ansatz basis. We focus on constructing scattering states where the incoming particles are a free Fermi-sea at zero temperature. Such scattering states, using a conjecture discussed below, allow one to recover the zero temperature thermodynamics of the Kondo model using scattering states.

It was shown earlier that for scattering states with the asymptotic boundary conditions that the incoming particles are a Fermi sea, that the scattering state $|\Psi\rangle$ can be

described by a single Bethe-Ansatz wavefunction. The most general Bethe-Ansatz wavefunctions is of the form

$$|\Psi\rangle = \int d\vec{x}\, e^{\sum_j p_j x_j} \sum_Q S^Q A_{\alpha_1 \ldots \alpha_N \alpha_0} \theta(x_Q) \prod_{j=1}^{N} \psi^\dagger_{\alpha_j}(x_j)|0\rangle. \tag{64}$$

with S^Q the product of two-particle S-matrices in the Kondo model, $S^{ij} = P^{ij}$ for electron-electron scattering and $S^{i0} = \frac{1+iJP^{i0}}{1+iJ}$ for electron impurity scattering with P^{ij} is the permutation matrix that exchanges the spins of particles i and j[21].

The asymptotic boundary conditions that the incoming particles be a filled Fermi-sea now reduce to choosing the Bethe-Ansatz momenta $\{p_j\}$ and the amplitude $A_{\alpha_1 \ldots \alpha_N \alpha_0}$ so that when all the particles are to the left of the impurity are scattering state reduces to eigenstate of H_0 in the Kondo Bethe-Ansatz basis describing a filled Fermi-sea. This state, $|\Phi\rangle_{baths}$ is extensively discussed in the appendix and is described by a wavefunction of the form (A10) with $A_{b_1 \ldots b_N}$ given by (A13)and BA momenta $\{p_j\}$ of the form $\frac{2\pi n_j}{L}$ with n_j integers running from $-N$ to 0. The amplitude is written in terms of solutions to (A12), the spin rapidities $\{\Lambda_\gamma\}$.

When all particles are to the left of the impurity, the scattering state (64) reduces to

$$|\Psi\rangle \rightarrow \tag{65}$$
$$\int d\vec{x}\, e^{\sum_j i p_j x_j} \sum_{Q'} S^{Q'} A_{\alpha_1 \ldots \alpha_N \alpha_0} \theta(x_{Q'}; x_0) \prod_{j=1}^{N} \psi^\dagger_{\alpha_j}(x_j)|0\rangle.$$

with Q' a permutation of the N^e electrons, $\theta(x_{Q'}; x_0) = \theta(x_{Q'(1)} < \theta_{Q'(2)} < \ldots < x_{Q'(N^e)} < x_o)$ with x_0 the position of the impurity. Since reaching the regions Q' involves no electron-impurity scattering, the S^Q is a product of the electron-electron scattering matrix $S^{ij} = P^{ij}$ only. If we choose the momenta $\{p_j\}$ and amplitude $A_{b_1 \ldots b_N}$ as in the paragraph above, (**??**) reduces to the desired eigenstate of H_0 (A10). Thus, the imposition of the boundary-conditions follows directly from the representation of the filled Fermi-sea in the Kondo Bethe-Ansatz basis.

Summarizing, the full scattering state is described by (**??**) with the additional conditions that $A_{b_1 \ldots b_N}$ be of the form (A13) with the $\{\Lambda_\gamma\}$ solutions to (A12) whose density is given by (A16) and BA momenta $\{p_j\}$ of the form $\frac{2\pi n_j}{L}$ with n_j integers running from $-N$ to 0. Choosing the amplitude and BA momenta in this way ensure the scattering state $|\Psi\rangle$ reduces to a state describing a filled Fermi sea $|\Phi\rangle_{baths}$ for incoming particles.

B. Can we map the Kondo to an abelian quantum-impurity problem?

Having constructed the scattering state, the next task is to compute quantum-impurity properties using this state. This task is significantly more difficult than in the IRLM since the amplitude $A_{b_1 \ldots b_N}$ is written in terms of lowering B operators of the quantum-inverse scattering method. These operators do non commute but instead satisfy a complicated algebra. This makes it difficult to manipulate them[21]. For this reason, it is quite desirable to explore the intriguing possibility that the Kondo problem is in fact equivalent to an auxiliary quantum-impurity problem similar to the IRLM. The central difference between the Kondo scattering state and the IRLM is that the scattering states for the Kondo problem are constructed using non-abelian two particle S-matrices where as the two-particle S-matrix for the IRLM is an abelian phase. We call models with abelian two-particle S-matrices, abelian quantum impurity problems. In this section, we conjecture that the Kondo problem can indeed be mapped to a very particular 'abelian' quantum-impurity problem. This abelian quantum-impurity problem correctly reproduces the thermodynamics of the Kondo model. We conjecture that arguments similar to those given by Maillet et al will show that the abelianization of the problem extends to all quantities allowing an easy computation of the scattering properties.

The starting point for the conjecture are the Bethe-Ansatz equations for the Kondo model. These Bethe-Ansatz equations are derived using the TBA by considering a quantum impurity on a finite ring of length L and imposing periodic boundary conditions. They are given by

$$\begin{aligned} e^{ip_j L} &= \textstyle\prod_{\gamma=1}^{M} \frac{\Lambda_\gamma - 1 + ic/2}{\Lambda_\gamma - 1 + ic/2} \\ \prod_{\delta=1, \delta\neq\gamma}^{M} \frac{\Lambda_\delta - \Lambda_\gamma + ic}{\Lambda_\delta - \Lambda_\gamma - ic} &= \left(\tfrac{\Lambda_\gamma - 1 - ic/2}{\Lambda_\gamma - 1 + ic/2}\right)^{N^e} \left(\tfrac{\Lambda_\gamma - ic/2}{\Lambda_\gamma + ic/2}\right)^{N^i} \end{aligned} \tag{66}$$

with the additional information that the energy of the Bethe-Ansatz wavefunction is $E = \sum_j p_j$. The Λ are known as the spin rapidity and parameterize the M spin-down particles. We also need the log of these equations which yields

$$\begin{aligned} p_j &= \frac{2\pi}{L} n_j + \frac{1}{L} \sum_{\gamma=1}^{M} [\theta_2(\Lambda_\gamma - 1) - \pi] \\ N^e \theta_2(\Lambda_\gamma - 1) &+ N^i \theta_2(\Lambda_\gamma) = -2\pi I_\gamma + \sum_{\delta=1}^{M} \theta_1(\Lambda_\gamma - \Lambda_\delta) \end{aligned} \tag{67}$$

with $\theta_n(x) = -2\tan^{-1} nx/c$ and n_j and I_j integers coming from the logarithm and are the charge and spin quantum numbers respectively. The energy of the eigenstate

is given

$$\begin{aligned} E &= \sum_j p_j = \sum_j \frac{2\pi}{L} n_j + \frac{N^e}{L} \sum_{\gamma=1}^{M} \left[\theta_2(\Lambda_\gamma - 1) - \pi\right] \\ &= \sum_j \frac{2\pi}{L} n_j + \frac{1}{L} \sum_{\gamma=1}^{M} \left[-2\pi I_\gamma - N^i \theta_2(\Lambda_\gamma) + \sum_{\delta=1}^{M} \theta(\Lambda_\gamma - \Lambda_\delta) \right] \\ &= \sum_j \frac{2\pi}{L} n_j + \sum_{\gamma=1}^{M} -\frac{2\pi}{L} I_\gamma + \frac{N^i}{L} \sum_{\gamma=1}^{M} -\theta_2(\Lambda_\gamma) \end{aligned} \tag{68}$$

The first two terms are the energy of a free-electron gas in the spin-charge decoupled Kondo basis and the last term is the shift in the ground state energy due to the Kondo impurity. Previously, we have defined this as the impurity energy E_{imp}. Thus, for the Kondo problem we can write (suggestively)

$$E_{imp} = \frac{1}{L} \sum_{j=1}^{M} \delta_K(\Lambda_\gamma) \tag{69}$$

with $\delta_K(\Lambda) = -\theta_2(\Lambda_\gamma) = 2\tan^{-1}(2\Lambda/c)$. We can also define a phase $\Phi_K(\Lambda_\gamma - \Lambda_\delta) = \theta_1(\Lambda_\gamma - \Lambda_\delta)$ and a function $\tilde{k}(\Lambda) = D\theta_2(\Lambda - 1)$ with $D = N^e/L$. Then, the second Bethe-Ansatz equation in(67) can be derived from the equation

$$e^{i\tilde{k}(\Lambda_\gamma)L} = e^{i\delta_K(\Lambda_\gamma)} \prod_{\delta=1}^{M} e^{i\Phi_K(\Lambda_\gamma - \Lambda_\delta)}$$

by taking the natural logarithm of both sides. This suggestive notation is illuminating because the above equation is of the form of the self-consistency monodromy equation in the TBA that leads to the BAE

$$e^{i\tilde{k}(\Lambda)L} A = Z_j A = \left(S^{jj-1} \dots S^{j1} \dots S^{jM} S^{j0} \dots S^{jj+1}\right) A$$

with $S^{js} = e^{i\Phi_K(\Lambda_j - \Lambda_s)}$ $(j, s \neq 0)$ and $S^{j0} = e^{i\delta_K(\Lambda_\gamma)}$.

Thus, viewing the $\Lambda' s$ as a function of the $\tilde{k}' s$, we see that the BAE for the Kondo problem could be derived from another abelian quantum impurity problem of M electrons with an electron-electron scattering matrix given by $S^{js} = e^{i\Phi_K(\Lambda_j - \Lambda_s)}$ and electron-impurity scattering matrix given by $S^{j0} = e^{i\delta_K(\Lambda_\gamma)}$.

The SBA can be applied to this auxiliary quantum-impurity problem in the abelian formulation. The scattering states are analogous to those of the IRLM model with $\{\Phi, \delta\} \to \{\Phi_K, \delta_K\}$. A straight-forward construction and calculation using the SBA for this abelian problem yield the correct Kondo thermodynamic properties. This opens up the possibility that scattering properties of the Kondo model can be alternatively calculated in this abelian quantum-impurity model where manipulations of the scattering states are much easier. The scattering states constructed in the last section are unwieldily because they are defined in terms of complicated algebras found in the ABA.

The open problem in this conjecture is how to map operators in the original Kondo problem to this new abelian quantum-impurity problems. Such a mapping has been worked out for the Heisenburg spin-chain by Terras and collaborators[27]. Due to the close analogy of the Bethe-Ansatz equations for the Heisenburg spin chain equations, we expect that a similar mapping of operators can be performed for the Kondo model. If such a mapping can be fully flushed out, the SBA should lead to exact solutions for many impurity properties such as the impurity T and S-matrices.

VII. CONCLUSIONS

This paper outlines a scattering framework for quantum-impurity models. Generally, constructing scattering states for interacting impurity models is quite difficult. However, if the model is integrable, these states can be constructed using the Scattering Bethe Ansatz developed in this paper. The SBA correctly reproduces the zero temperature thermodynamic properties of both the Kondo model and the IRLM. In addition, it raises the exciting possibility that the Kondo model may be equivalent to an abelian quantum-impurity problem.

The scattering framework also gives us insight into how the Bethe-Ansatz works. The impurity physics in any Bethe-Ansatz basis, always looks like single-particle impurity phase shifts, δ. This suggests that the Bethe-Ansatz basis diagonalizes the lead electrons so that the impurity T-matrix is a phase shift. The complexity of the problem is shifted from the impurity-electron interaction to finding an appropriate basis for free electrons. This observation is essential when using the SBA to calculate nonequilibrium properties of the Kondo model. We feel that this new perspective on the Bethe-Ansatz may lead to new physical insights and is worth exploring in greater detail.

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APPENDIX A: THE BETHE-ANSATZ BASIS FOR KONDO AND IRLM

In general constructing scattering eigenstates is a formidable task. However, for integrable quantum-impurity models such as the IRLM and Kondo Models, scattering states can be constructed using a generalization of the Algebraic Bethe-Ansatz and quantum Inverse scattering methods. Consequently, the natural basis for these scattering states is not the Fock basis, but rather a

new 'Bethe-Ansatz' basis. Central to constructing scattering eigenstates, is the requirement that far away for the impurity, the incoming electrons look like a free Fermi sea. In this section, we show how to represent a Fermi-sea in the Bethe-Ansatz basis appropriate to the IRLM and Kondo models. For these models, the impurity forces two-particle S-matrices S^{ij} to be[21,26]

$$\begin{aligned} S_{IRLM} &= e^{i\Phi(p_i,p_j)} = \exp\left(i\tan^{-1}\left(\frac{U(p_i-p_j)}{2(p_i+p_j-2\epsilon_d)}\right)\right) \\ S^{ij}_{Kondo} &= P^{ij} \end{aligned} \tag{A1}$$

In this appendix we show how to represent free-electrons in the Bethe-Ansatz basis for each of these models. Denote these two-basis the IRLM basis and the Kondo basis respectively.

1. Free Electrons in the IRLM Bethe-Ansatz Basis

We first focus on the IRLM. Particles in the IRLM are spinless and labelled by their B.A. momenta p_j. The IRLM Bethe-Ansatz basis has a electron-electron S-matrices of the form (A1). A Bethe-Ansatz wavefunction in the IRLM Bethe-Anatz basis is given by (up to an overall multiplicative phase independent of the $\{x_j\}$)

$$\begin{aligned} |N, BA\rangle &= A\int d\vec{x} e^{i\sum_j p_j x_j} e^{\frac{i}{2}\sum_{i<j} sgn(x_i-x_j)\Phi(p_i,p_j)} \\ &\quad \psi^\dagger(x_1)\dots\psi^\dagger(x_N)|0\rangle. \end{aligned} \tag{A2}$$

with $sgn(x)$ the sign function which is equal to ± 1 if $x > 0/x < 0$. In writing the above expression, we have used the identity that $(\theta(-x) + e^{i\Phi}\theta(x)) = e^{-i\frac{i}{2}\Phi} e^{\frac{i}{2}\Phi sgn(x)}$. As discussed in the main text, to find the B.A. momenta $\{p_j\}$ we consider an auxiliary problem of free electrons living on a finite ring of size L'. In the $L' \to \infty$ the momenta of the physical and auxiliary problem coincide.

We restrict ourselves to the zero temperature case and when ϵ_d is greater than the Fermi-level of the electrons. This is the case considered in[26]. To derive the Bethe-Ansatz for the BA momenta distribution functions, we must equate the wavefunction for the auxiliary problem on a circle when a particle j is at $x_j = 0$ and at $x_j = L'$. This gives rise to a Bethe-Ansatz condition of the form

$$S^{1j}\dots S^{j-2j} S^{j-1j} A = S^{jN}\dots S^{jj+1} e^{ip_j L'} \tag{A3}$$

which implies that

$$\left(S^{jj-1}\dots S^{j1} S^{jN}\dots S^{jj+1}\right) A = e^{-ip_j L'} A. \tag{A4}$$

Plugging in the explicit form of the two-particle S-matrix for the IRLM from (A1), this equation gives rise to an equation for the BA momenta $\{p_j\}$ of the form (noting that we can cancel A from both sides since it is a constant)

$$e^{ip_j L'} = e^{i\sum_{s=1}^N \Phi(p_j,p_s)}. \tag{A5}$$

Taking the log and multiplying by $-i$ one has

$$p_j = \frac{1}{L'}\sum_{s=1}^N \Phi(p_j,p_s) + \frac{2\pi n_j}{L'} \tag{A6}$$

with n_j an integer. Notice that the amplitude A has dropped out of the equation implying that it may be taken to be any constant. Notice that the 'free' Bethe-Ansatz equations (A6) for the BA momenta of H_0 in the IRLM basis can be obtained form the Bethe-Ansatz equations for the full IRLM Hamiltonian (including impurity interactions)[26]

$$p_j = \frac{1}{2L'}\sum_{s=1}^N \Phi(p_j,p_s) + \frac{2\pi n_j}{L'} + \frac{N^i}{L'}\delta_p, \tag{A7}$$

by setting the impurity contribution proportional to N^i equal to zero.

As is usual, we will not be concerned with solving the discrete version of this equation but instead will solve for the distribution function, $\rho(p)$ describing the density of solutions to the equations in an interval $(p, p+dp)$. It is worth emphasizing that such distributions make sense only in the limit $L' \to \infty$. In this limit, we can replace the sum by an integral to get

$$p_j = \int dk \rho(k)\Phi(p_j,k) + \frac{2\pi n_j}{L'}. \tag{A8}$$

In the usual way, an equation for the zero temperature density $\rho(p)$ is obtained by subtracting the equation for p_j from that for p_{j+1} and expanding in the difference $\Delta p = p_{j+1} - p_j$ which yields[21]

$$\begin{aligned} \rho(p) &= \frac{1}{2\pi} - \int dk \rho(k) K(p,k) \\ K(p,k) &= \frac{1}{2\pi}\frac{\partial\Phi(p,k)}{\partial p} = \frac{U}{\pi}\frac{(k-\epsilon_d)}{(p+k-2\epsilon_d)^2 + \frac{U^2}{4}(p-k)^2} \end{aligned} \tag{A9}$$

This equations are valid as long as ϵ_d is greater than the Fermi energy of the lead electrons. Though we do not do it here, we could also find the distribution of the BA momenta at finite temperatures by considering the free Thermodynamic Bethe Ansatz (TBA) equations for H_0 corresponding to the free zero temperature BA equation (A9) for H_0.

Summarizing, in the IRLM basis, there is a non-trivial two particle S-matrix between free electrons of the form (A1). The presence of this matrix corresponds to working in a Bethe-Ansatz basis for the IRLM that is distinct from the usual Fock basis. In this basis, the eigenstates of H_0 are of the form (A2) with the multi-particle S-matrices S^Q given as products of two particle S-matrices of the form (A1). For a free Fermi-sea at zero temperature, the distribution for the BA momenta, $\rho(p)$, is given by (A9) not the Fermi-Dirac distribution functions.

2. Free Electrons in the Kondo Bethe-Ansatz Basis

We now concentrate of the wavefunction of a free-Fermi sea at zero temperature in the Kondo basis. In the Kondo basis, free-electrons have a two-particle S-matrix $S^{ij} = P^{ij}$ where P^{ij} is the permutation matrix acting on the spins of electrons i and j[21]. The Bethe-Ansatz wavefunction for the Kondo Bethe-Ansatz basis is

$$|N\rangle = \int d\vec{x} e^{i\sum_j p_j x_j} (S^Q)^{b_1\ldots b_N}_{a_1\ldots a_N} A_{b_1\ldots b_N} \theta(\vec{x}_Q) \quad \text{(A10)}$$
$$\psi^\dagger_{a_1}(x_1)\ldots\psi^\dagger_{a_N}(x_N)|0\rangle$$

with S^Q an appropriate product of two particle S-matrices P^{ij}. Note that the amplitude in the region $Q = 1$, $A_{b_1\ldots b_N}$ and the choice of BA momenta $\{p_j\}$ are still unspecified. We will once again have to choose these appropriately by considering an auxiliary problem defined on a circle of length L'. In the limit where $L' \to \infty$, the expressions from the auxiliary problem coincide with those for the infinite-size open system. Thus, we can use the beautiful quantum-inverse scattering technology[21].

Once again the BA equations for the auxiliary problem are derived by equating the wavefunction for the auxiliary problem on a circle when a particle j is at $x_j = 0$ and at $x_j = L'$. This gives rise to a Bethe-Ansatz condition of the form

$$(Z_j)^{b_1\ldots b_N}_{a_1\ldots a_N} A_{b_1\ldots b_N} = \quad \text{(A11)}$$
$$\left(S^{jj-1}..S^{j1}S^{jN}..S^{jj+1}\right)^{b_1\ldots b_N}_{a_1\ldots a_N} A_{b_1\ldots b_N} = e^{-ip_jL'} A_{a_1\ldots a_N}.$$

We must choose $A_{b_1\ldots b_N}$ such that it is eigenvector for the equation $Z_j A = z_j A$ with eigenvalue $z_j = e^{-ip_jL}$. Note, that in general there are many solutions to this equation. We will be concerned with a single eigenvector, namely the ground-state.

A general method called the quantum-inverse scattering method has been developed to solve this problem. Let N and M denote the total number of particles and the total number of spin down particles respectively. Let us denote the spin Hilbert space of particle j by V_j. Let $V^N \otimes \prod_{j=1}^N V_j$ be the N-particle spin-space. The Bethe-Ansatz equations for the ferromagnetic vacuum are[21]

$$z_j = \lambda(\alpha_j, \beta_1\ldots\beta_M) = \prod_{\gamma=1}^{M} \frac{\Lambda_\gamma + i\frac{c}{2}}{\Lambda_\gamma - i\frac{c}{2}}$$
$$\prod_{\delta=1,\delta\neq\gamma}^{M} \frac{\Lambda_\delta - \Lambda_\gamma + ic}{\Lambda_\delta - \Lambda_\gamma - ic} = \left(\frac{\Lambda_\gamma - i\frac{c}{2}}{\Lambda_\gamma + i\frac{c}{2}}\right)^N \quad \text{(A12)}$$

Each set of solutions to the Bethe-Ansatz equations $\{\lambda_j\}$ corresponds to a different eigenstate of H_0. Different choices of M correspond to eigenstates of spin $N/2 - M$. Since, We are interested in the ground state configuration with zero spin we restrict ourselves to the sector where $M = \frac{N}{2}$. Let the solutions of the BA equations with $M = N/2$ for the ground state be given by $\{\Lambda^{gs}_j\}$. Define $\beta_\gamma = \Lambda^{gs}_\gamma + ic$ and denote the ferromagnetic vacuum in the space V^N by $|\omega\rangle = \prod_{j=1}^N \begin{pmatrix} 1 \\ 0 \end{pmatrix}_j$. Then, the amplitude $A_{b_1\ldots b_N}$ in (A10) is given by

$$A(\Lambda_1\ldots\Lambda_M)_{b_1\ldots b_N} = B(\Lambda_1 + ic/2)\ldots B(\Lambda_M + ic/2)|\omega\rangle$$
$$= \sum_{j_1\ldots j_M} A_{j_1\ldots j_M} \sigma^-_{j1}\ldots\sigma^-_{j_M}|\omega> \quad \text{(A13)}$$

where the usual spin amplitude notation $A_{b_1\ldots b_M}$ is written as $A_{j_1\ldots j_M}$ by specifying the position of the M down spins and the operators $B(\Lambda_\gamma + ic/2)$ are defined in the as is usual in the quantum-inverse scattering matrix[21]. The B are best thought of as generalized lowering operators σ^- that lower the spin of particle j. The BA momenta $\{p_j\}$ in (A10) on the other hand are trivially of the from $p_j = \frac{2\pi n_j}{L}$. For the ground state, it runs from some lower cut-off $K = -\frac{2\pi N}{L}$ to the Fermi energy at zero.

Just as in the IRLM case, we can talk about the density of $\{\lambda_j\}$, $\sigma_o(\lambda_j)$ rather than the individual λ themselves. This approach is valid in the limit: $N, L \to \infty$ with $D = N/L$ held fixed. To get the distribution for the density, we take the logarithm of both sides of the second equation in (A12) to get

$$N^e\theta(2\Lambda_\gamma) = -2\pi I_\gamma + \sum_{\delta=1}^{M} \theta(\Lambda - \Lambda_\gamma) \quad \text{(A14)}$$

with $\theta(x) = -2\tan^{-1}(x/c)$ and I_γ an integer. Since we are interested in the $\{\lambda_j\}$ for the groundstate, we set $M = N/2$. We then consider $\sigma_o(\Lambda)$ describing the number of solutions in an interval $(\Lambda, \Lambda + d\Lambda)$. Standard manipulations yield the equation[21]

$$\sigma_o(\Lambda) = \frac{2c}{\pi}\left[\frac{N}{c^2 + 4\Lambda^2}\right] - \frac{1}{\pi}\int d\Lambda' \sigma_o(\Lambda') K(\Lambda - \Lambda')$$
$$K(\Lambda) = \frac{1}{\pi}\frac{c}{c^2 + \Lambda^2}. \quad \text{(A15)}$$

This can be easily solved by Fourier transform to yield the equation for the density of $\{\lambda_j\}$ in the groundstate,

$$\sigma_o(\Lambda) = \frac{1}{2c}\frac{N}{\cosh\frac{\pi}{c}\Lambda}. \quad \text{(A16)}$$

To summarize, a Free Fermi sea in the Kondo Bethe-Ansatz basis is captured by a state of the form (A10) with $A_{b_1\ldots b_N}$ given by (A13), the $\{\Lambda_\gamma\}$ solutions to (A12) whose density is given by (A16). The BA momenta $\{p_j\}$ are of the trivial

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