Nonequilibrium Transport in Quantum Impurity Models: The Bethe Ansatz for Open Systems

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We develop an exact nonperturbative framework to compute steady-state properties of quantum impurities subject to a finite bias. We show that the steady-state physics of these systems is captured by nonequilibrium scattering eigenstates which satisfy an appropriate Lippman-Schwinger equation. Introducing a generalization of the equilibrium Bethe ansatz—the nonequilibrium Bethe ansatz—we explicitly construct the scattering eigenstates for the interacting resonance level model and derive exact, nonperturbative results for the steady-state properties of the system.

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The recent spectacular progress in nanotechnology has made it possible to study quantum impurities out of equilibrium [1]. The impurity is typically realized experimentally as a quantum dot, a tiny island of electron liquid attached via tunnel junctions to two leads (baths or reservoirs) held at different chemical potentials. As a result of the potential difference, an electric current flows from one lead to another across the quantum impurity. The description of such an out-of-equilibrium situation in a strongly correlated system is a long-standing problem and has not been given even in the simplest case of when the system is in a steady state.

In a steady state, the system properties do not change with time even when out of equilibrium. Such a state is reached only under special conditions: Each lead needs to be a good thermal bath and infinite in size (equivalently, the bath level spacing tends to zero). It then follows that particles transferred from one lead to another dissipate their extra energy in the lead and equilibrate [2].

There are two equivalent ways, time-dependent and time-independent, to describe the establishment of a steady state in the system. In the time-dependent picture, the quantum impurity is coupled to the two baths in the far past t_0 and is allowed to evolve adiabatically under the conditions described above. After a sufficiently long time, at $t = 0$, say, a steady state is reached. Two elements are required to fully determine the system: a Hamiltonian to describe the time evolution and an initial condition ρ_0 describing the system in the far past. The Hamiltonian is chosen to be of the form $H(t) = H_0 + e^{\eta t} H_1$, where H_0 describes the two free leads (thermal baths), H_1 is the interaction term between the leads and the quantum impurity, and η is an infinitesimal parameter, small enough to ensure adiabaticity, yet large compared to the level spacing in the leads. The initial condition is typically given by

$$\rho_0 = \frac{e^{-\beta(H_0 - \sum_i \mu_i N_i)}}{\mathrm{Tr} e^{-\beta(H_0 - \sum_i \mu_i N_i)}}, \tag{1}$$

with μ_i and N_i the chemical potential and number operator for particles in lead i, respectively. Subsequently, at times $t \geq t_0$, the system is described by a density matrix $\rho(t) = T\{e^{i\int_{t_0}^{t} dt' H(t')}\}\rho_0 T\{e^{-i\int_{t_0}^{t} dt' H(t')}\}$, and the properties of the system are calculated in the usual manner, $\langle \hat{O}(t) \rangle = \mathrm{Tr}\{\rho(t)\hat{O}\}$. The establishment of a steady state follows, in this language, from the existence of the limit $t_0 \to -\infty$ with the expectation value becoming time-independent, $\langle \hat{O} \rangle = \mathrm{Tr}\{\rho_s \hat{O}\}$, where $\rho_s = \rho(0)$.

At $T = 0$, the description simplifies. The initial condition is typically given by a particular eigenstate of H_0, $|\Phi\rangle_{\mathrm{baths}}$, describing the baths, each with its own chemical potential μ_i. The steady state is then obtained by evolving the initial state in time, $|\Psi\rangle_s = T\{e^{i\int_{-\infty}^{t} dt' H(t')}\}|\Phi\rangle_{\mathrm{baths}}$. The expectation values in the steady state are computed from

$$\langle \hat{O} \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle_s}{\langle \Psi | \Psi \rangle_s}. \tag{2}$$

An equivalent way to describe a nonequilibrium steady state is by means of a time-independent scattering formalism. The state $|\Psi\rangle_s$ is obtained as an eigenstate of the full Hamiltonian $H = H_0 + H_1$, satisfying the Lippman-Schwinger equation,

$$|\Psi\rangle_s = |\Phi\rangle_{\mathrm{baths}} + \frac{1}{E - H_0 + i\eta} H_1 |\Psi\rangle_s, \tag{3}$$

with $|\Phi\rangle_{\mathrm{baths}}$—the incoming state. The scattering eigenstate $|\Psi\rangle_s$ can be viewed as consisting of incoming particles (the two free Fermi seas) described by $|\Phi\rangle_{\mathrm{baths}}$ and reflected outgoing particles given by the second term in the above equation. Once again, two elements are required to fully determine the system: a Hamiltonian and a boundary condition $|\Phi\rangle_{\mathrm{baths}}$, which describes the scattering state far from the impurity. Note that, previously, in the time-dependent picture, $|\Phi\rangle_{\mathrm{baths}}$ played the role of an initial condition rather than a boundary condition.

The construction of such eigenstates is a formidable task, in general. We shall show, however, that it can be carried out for a class of integrable impurity models that includes the interacting resonance level model (IRLM) and

the Kondo model. The Bethe-ansatz solution of these integrable models in equilibrium has led to a full understanding of their thermodynamic properties. It is based on solving the Hamiltonian of a closed system, typically with periodic boundary conditions. We shall present in this Letter a significant generalization of the Bethe-ansatz approach to *open systems* with boundary conditions imposed by the leads. This approach, the nonequilibrium Bethe ansatz, allows us to construct the fully interacting multiparticle scattering eigenestates and compute nonequilibrium transport properties, extending Landauer's original approach [3]. We remark here that our approach differs significantly from the recent interesting work by Konik *et al.* [4], who also used integrability to compute transport. In contrast to their work, we model the leads as free Fermi seas rather than coupling the chemical potentials to dressed excitations.

We focus on the IRLM and defer treatment of other models to later publications. The IRLM $H_{\mathrm{IRL}} = \sum_{i=1,2,\vec{k}} \epsilon_k \psi^\dagger_{i\vec{k}} \psi_{i\vec{k}} + \epsilon_d d^\dagger d + \frac{t}{\sqrt{2}} \sum_{i=1,2,\vec{k}} (\psi^\dagger_{\vec{k}} d + \mathrm{H.c.}) + 2U \sum_{i=1,2,\vec{k},\vec{k}'} \psi^\dagger_{i\vec{k}} \psi_{i\vec{k}'} d^\dagger d$ describes a resonant level $\epsilon_d d^\dagger d$ coupled to two baths of spinless electrons via tunneling junctions with strength t. There is also a Coulomb interaction U between the level and the baths. The model is closely related to the anisotropic Kondo model [5], with the charge states $n_d = 0, 1$ playing the role of spin states and ϵ_d playing the role of a local magnetic field.

Performing some standard manipulations for impurity models, expanding in angular modes around the impurity, keeping only the s modes, unfolding the model, and linearizing around the two Fermi points, we have

$$H_{\mathrm{IRL}} = -i \sum_{i=1,2} \int dx \psi^\dagger_i(x) \partial \psi_i(x) + \epsilon_d d^\dagger d + \frac{t}{\sqrt{2}} \left[\sum_{i=1,2} \psi^\dagger_i(0) d + \mathrm{H.c.} \right] + 2U \sum_{i=1,2} \psi^\dagger_i(0) \psi_i(0) d^\dagger d. \quad (4)$$

The model thus obtained is a renormalizable field theory which requires introduction of a cutoff procedure to render it finite. The values of the bare parameters U, ϵ_d, t will be renormalized as the cutoff is removed to yield a physical theory. The renormalized theory captures the universal physics—where voltages and temperatures are small compared to the cutoff (bandwidth D). The chemical potentials for the leads are not included in the Hamiltonian. Instead, they enter as nonequilibrium boundary conditions specifying the scattering state far from the impurity.

We wish to calculate the expectation values in the steady state of the dot occupation $\hat{n}_d = d^\dagger d$ and the current operator $\hat{I} = \frac{i}{2} \sum_{j=1,2} (-1)^j t/\sqrt{2} [\psi^\dagger_j(0) d - \mathrm{H.c.}]$, the latter deduced from $\hat{I} = \frac{1}{2}[(N_1 - N_2), H]$.

To construct the scattering states, we use a new Bethe-ansatz technique, which, unlike the traditional approach based on closed systems and periodic boundary conditions, allows the determination of a state by boundary conditions imposed asymptotically. The many-body scattering state is built using single-particle scattering states that incorporate the boundary conditions. Introducing a symmetric/antisymmetric basis defined by $\psi_{e/o}(x) = \frac{1}{\sqrt{2}}[\psi_1(x) \pm \psi_2(x)]$, the Hamiltonian separates into even and odd parts: $H_e = -i \int dx \psi^\dagger_e(x) \partial \psi_e(x) + U \psi^\dagger_e(0) \psi_e(0) d^\dagger d + t[\psi^\dagger_e(0) d + \mathrm{H.c.}] + \epsilon_d d^\dagger d$ and $H_o = -i \int dx \psi^\dagger_o(x) \partial \psi_o(x) + U \psi^\dagger_o(0) \psi_o(0) d^\dagger d$. The boundary conditions, however, are imposed in the physical basis $\psi_{1/2}$, requiring appropriate combinations of both the even and odd sectors. The single-particle eigenstates of the model are

$$\int dx \{A[g_p(x) \psi^\dagger_e(x) + e_p d^\dagger] + B h_p(x) \psi^\dagger_o(x)\} |0\rangle, \quad (5)$$

with $|0\rangle$ the empty vacuum and A and B arbitrary constants chosen to satisfy the nonequilibrium boundary conditions. We are interested in two solutions, labeled $\pm$, to the Schrödinger equation for these eigenstates,

$$\begin{aligned} g_p(x) &= \frac{2e^{ipx}}{1 + e^{i\delta_p}} [\theta(-x) + e^{i\delta_p} \theta(x)], \qquad [g_p(0) = 1], \\ h^\pm_p(x) &= \frac{2e^{ipx}}{1 + e^{i\delta_p}}, \qquad x \neq 0, \\ h^\pm_p(0) &= \pm (p - \epsilon_d)(e_p/t) e^{ipx} = \pm g_p(0) e^{ipx}, \qquad x = 0, \end{aligned} \quad (6)$$

with $e_p = t g_p(0)/(p - \epsilon_d)$ and $\delta_p = 2 \arctan[t^2/2(p - \epsilon_d)]$. Note that we take $h_p(x)$ to be discontinuous at zero. This unorthodox choice of solution is allowed by the linear derivative. Theories with linear derivatives are implicitly many-body theories, and to calculate their physical observables one must first fill the Fermi sea from a lower cutoff $(-D)$ to the Fermi energy, as we do below.

We construct two kinds of single-particle scattering states, namely, those with incoming particles from lead 1, $|1p\rangle$, and those with incoming particles from lead 2, $|2p\rangle$, with p the momentum of the incoming particle. Choosing $A = B$ in Eq. (5), the amplitude for an incoming particle from lead 2 vanishes, and we get

$$|1p\rangle = \int dx e^{ipx} \left[\frac{2}{1 + e^{i\delta_p}} \{[2\theta(-x) + (e^{i\delta_p} + 1)\theta(x)] \psi^\dagger_1 + [(e^{i\delta_p} - 1)\theta(x)] \psi^\dagger_2\} + \sqrt{2} e_p d^\dagger \delta(x) \right] |0\rangle.$$

Conversely, choosing $A = -B$, the amplitude for an incoming particle from lead 1 vanishes and we get the state $|2p\rangle$, given by the above expression with $\psi^\dagger_1(x)$ and $\psi^\dagger_2(x)$ interchanged. It is convenient to introduce the operators $\alpha^\dagger_{1/2p}(x) = g_p(x) \psi^\dagger_e(x) \pm h^\pm_p(x) \psi^\dagger_o(x) + e_p \delta(x) d^\dagger$, in terms of which the scattering states are $|1/2p\rangle = \int dx e^{ipx} \alpha^\dagger_{1/2p}(x) |0\rangle$. The single-particle scattering eigenstates are depicted in Fig. 1.

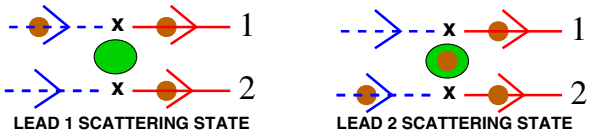

FIG. 1 (color online). There are two types of single-particle scattering states. In a type 1 scattering state, an incoming electron in lead 1 is scattered by the impurity and can hop onto either lead 1 or lead 2.

The two-particle eigenfunction is of the form

$$\int [Ag(x_1,x_2)\psi_e^\dagger(x_1)\psi_e^\dagger(x_2) + Ch(x_1,x_2)\psi_o^\dagger(x_1)\psi_o^\dagger(x_2) + Bj(x_1,x_2)\psi_e^\dagger(x_1)\psi_o^\dagger(x_2) + Ae(x)\psi_e^\dagger(x)d^\dagger + Bf(x)\psi_0^\dagger(x)d^\dagger]|0\rangle,$$

where

$$\begin{aligned} 2g(x_1,x_2) &= g_p(x_1)g_k(x_2)Z(x_1-x_2) - (1\leftrightarrow 2),\\ 2h(x_1,x_2) &= h_p(x_1)h_k(x_2)Z(x_1-x_2) - (1\leftrightarrow 2),\\ j^{ab}(x_1,x_2) &= g_p(x_1)h_k^a(x_2)Z(x_1-x_2)\\ &\quad + (-1)^{ab}g_k(x_1)h_p^b(x_2)Z(x_2-x_1), \end{aligned} \tag{7}$$

with $a, b = \pm$, $g_p(x)$ and $h_p^{a/b}(x)$ being the single-particle eignefunctions Eq. (6), and $Z(x_1-x_2) = e^{i\varphi(p,k)\mathrm{sgn}(x_1-x_2)}$, with: $e^{2i\varphi(p,k)} = (i + \{(U/2)[(p-k)/(k+p-2\epsilon_d)]\})/(i - \{(U/2)[(p-k)/(k+p-2\epsilon_d)]\})$. The constants A, B, and C are determined by the nonequilibrium boundary conditions. In this solution, we made use of freedom afforded by the linear dispersion to choose the two-particle S matrix between all electrons to be the same. This allows us to easily generalize the construction to N particle wave functions yielding the fully interacting scattering state

$$|\Psi\rangle_s = \int dx \Psi(x_1\cdots x_N)\prod_{u=1}^{N_1}\alpha_{1p_u}^\dagger(x_u) \times \prod_{v=N_1+1}^{N_1+N_2}\alpha_{2p_v}^\dagger(x_v)|0\rangle, \tag{8}$$

$$\Psi_s(x_1\cdots x_N) = e^{i\sum_j p_j x_j} e^{i\sum_{s<t}\varphi(p_s,p_t)\mathrm{sgn}(x_s-x_t)}.$$

Recall that, for $|\Psi\rangle_s$ to describe a nonequilibrium steady state, the incoming particles in the region $\{x_j\} \le 0$ must be described by $|\Phi\rangle_{\text{baths}}$. In the conventional Fock basis $|\Phi\rangle_{\text{baths}}$ is given by $\prod_{u=1}^{N_1} e^{i\sum_u \bar{p}_u x_u}\prod_{v=N_1+1}^{N_1+N_2} e^{i\sum_v \bar{p}_v x_v}$, with the Fock momenta $\{\bar{p}_j\}$ satisfying $-D \le \bar{p}_u \le \mu_1$ and $-D \le \bar{p}_v \le \mu_2$. Notice, however, that in $\Psi_s(x_1\cdots x_N)$ there is a two-particle S matrix, $S = e^{2i\varphi(p,k)}$, between incoming particles in each lead though the particles are free electrons. The presence of this nontrivial S matrix forces a choice of a different, "Bethe-ansatz," basis of eigenstates for the free Fermi seas in the leads, inherited from the interacting model when the coupling to the impurity is turned off. In order to impose the boundary condition in the Bethe-ansatz basis, the incoming particles Bethe-ansatz momenta $\{p_j\}$ in $|\Psi\rangle_s$, thus far undetermined, must be appropriately chosen. This is done below by solving "free-field" Bethe-ansatz equations.

The steady-state current and dot occupation in the nonequilibrium steady state is computed from Eq. (2) with $\hat{O}$ the appropriate operator and $|\Psi\rangle_s$ given by Eq. (8). When computing this expectation value, one must first take the system size L to infinity (recall that no steady state can be reached otherwise). In this limit, scattering states of types 1 and 2 are orthogonal and we find (denoting $\Delta = t^2/2$)

$$\begin{aligned} \langle I\rangle_s &= \sum_{u=1}^{N_1}\frac{\Delta^2}{(p_u-\epsilon_d)^2+\Delta^2} - \sum_{v=N_1+1}^{N_1+N_2}\frac{\Delta^2}{(p_v-\epsilon_d)^2+\Delta^2},\\ \langle n_d\rangle_s &= \sum_{u=1}^{N_1}\frac{\Delta}{(p_u-\epsilon_d)^2+\Delta^2} + \sum_{v=N_1+1}^{N_1+N_2}\frac{\Delta}{(p_v-\epsilon_d)^2+\Delta^2}. \end{aligned}$$

The apparent simplicity of these expressions may be misleading. The Bethe-ansatz structure of the wave functions transfers the complexity of the impurity interaction into the choice of Bethe-ansatz momenta $\{p\}$ for the incoming electrons, imposed by the nonequilibrium boundary conditions and the *interactions*. In the thermodynamic limit, this amounts to the determination of the Bethe-ansatz momenta distribution in each lead $\rho_i(p)$ $(i = 1, 2)$ through the solution of Bethe-ansatz equations arising from the presence of the nontrivial S matrix in (8). For $T = 0$, the distributions satisfy

$$\begin{aligned} \rho_1(p) &= \frac{1}{2\pi}\theta(k_o^1-p) - \sum_{j=1,2}\int_{-\infty}^{k_o^j}\mathcal{K}(p,k)\rho_j(k)dk,\\ \rho_2(p) &= \frac{1}{2\pi}\theta(k_o^2-p) - \sum_{j=1,2}\int_{-\infty}^{k_o^j}\mathcal{K}(p,k)\rho_j(k)dk, \end{aligned}$$

with k_o^i, $i = 1, 2$, upper bounds on the distributions of k, set by the chemical potentials μ_i (we choose $k_o^1 > k_o^2$), $\mathcal{K}(p,k) = \frac{U}{\pi}(k-\epsilon_d)/\{(p+k-2\epsilon_d)^2 + [(U^2/4)\times(p-k)^2]\}$. The equations need be solved in the presence of a cutoff D, $-D \le k$. Notice that the chemical potentials k_o^i come both in the limits of the integrals and in the driving terms $\theta(k_o^i - p)$. For $T > 0$, one needs to solve the corresponding finite temperature thermodynamic Bethe-ansatz (TBA) equations.

In terms of the distributions, the expressions for the current and the dot occupation become

$$\begin{aligned} \langle I\rangle_s &= \int dp[\rho_1(p)-\rho_2(p)]\frac{\Delta^2}{(p-\epsilon_d)^2+\Delta^2},\\ \langle n_d\rangle_s &= \int dp[\rho_1(p)+\rho_2(p)]\frac{\Delta}{(p-\epsilon_d)^2+\Delta^2}. \end{aligned} \tag{9}$$

For the noninteracting case, $U = 0$ implies $K(p,k) = 0$, and, hence, $\rho_i(p) = \frac{1}{2\pi}\theta(k_o^i - p)$—the product of the density of states $\nu = 1/2\pi$ and the Fermi-Dirac function at $T = 0$. Thus, (9) reverts to the standard $U = 0$ RL results [6]. In the $U = \infty$ limit, these equations can be solved by a standard, if tedious, Wiener-Hopf method, yielding

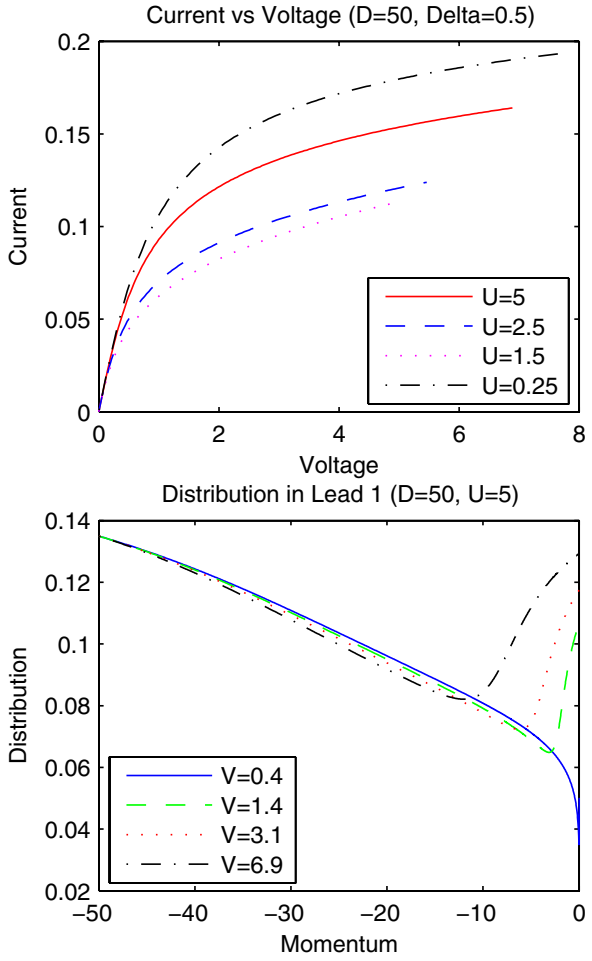

FIG. 2 (color online). Here we show the current as a function of voltage for various U with $\mu_{1/2} = \epsilon_d \pm V/2$ for fixed bandwidth D and Δ. Note that the current is not monotonic in U. We also show the distribution in lead 1 as a function of momentum for various voltages, where, without loss of generality, we take $k_o^1 = 0$.

the results: $\langle I\rangle_s = \frac{\Delta}{2\pi}(T_k/\Delta)\{\tan^{-1}[(\mu_1 - \epsilon_d)/T_k] - \tan^{-1}[(\mu_2 - \epsilon_d)/T_k]\}$ and $\langle n_d\rangle_s = \frac{1}{2} + \frac{1}{2\pi}(T_k/\Delta) \times \{\tan^{-1}[(\mu_1 - \epsilon_d)/T_k] + \tan^{-1}[(\mu_2 - \epsilon_d)/T_k]\}$, where $T_k = D(\frac{\Delta}{D})^{2\pi/\pi+\zeta}$ with $e^{i\zeta(U)} = (1 - [\frac{U}{2}]^2 + 2i\frac{U}{2})/(1 + [\frac{U}{2}]^2)$. T_k is a new low energy scale in the problem, related to the Kondo temperature in the anisotropic Kondo model. It is held fixed as the cutoff and U are sent to infinity.

More generally, these equations must be solved numerically with the bandwidth D much larger than all parameters in the problem to ensure we are in a universal regime. In Fig. 2, we plot our results for the current as a function of voltage for various values of U. Notice that the current is nonmonotonic in U with a duality between small and large U. This duality holds for all Δ. We also plot the distribution function in lead 1, ρ_1, as a function of momentum for various voltages. The nontrivial dependence on momentum and on voltage of these distributions is a hallmark of strongly correlated nonequilibrium physics.

As a stringent check on our approach, we examine the system for $\mu_1 = \mu_2$. The system reverts to equilibrium and our "open system" Bethe-ansatz construction can be confronted with the traditional "closed system" construction based on periodic boundary conditions. The dot occupation can be obtained in the latter approach from the impurity energy, given at zero temperature by $E_{\rm imp} = \int dp\rho(p)\delta_p$, with $\rho(p)$ determined by the standard TBA equation. Hence, ignoring $\partial_{\epsilon_d}\rho(p)$, which is suppressed by N/L, we have $\langle n\rangle_d = \partial_{\epsilon_d} E_{\rm imp} = \int dp\rho(p)\partial_{\epsilon_d}\delta_p$. Since $\partial_{\epsilon_d}\delta_p = 2\Delta/[(p - \epsilon_d)^2 + \Delta^2]$, it coincides with Eq. (9) when $\rho_1(p) = \rho_2(p) = \rho(p)$.

In conclusion, we have presented an exact solution of a strongly correlated impurity model out of equilibrium. The solution is given in terms of the scattering states that characterize the nonequilibrium steady state. The generalization to finite temperature or to more than two leads is straightforward. The latter allows the computation of the nonequilibrium density of states [7] which is of experimental interest. We believe the framework we introduced is very general and can be applied to most integrable models. Thus far, we have constructed current carrying scattering states for the Anderson and Kondo models, though we do not know a general criterion for the framework's applicability.

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