Quantum impurities in channel mixing baths

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The numerical renormalization group (NRG) is a powerful method for quantum impurity models. The success relies on the mapping of the effect of the conduction bath to the impurity into an open Wilson chain. However, with few exceptions, this is limited so far to the cases without channel mixing, leaving interesting cases, such as spin-orbital coupling, Cooper pairing and cluster impurity, largely beyond the scope of NRG. We fill the gap by a versatile scheme that maps a general channel-mixing bath into an open Wilson chain. After the comparison to a nontrivial known result, we apply the scheme for an Anderson impurity coupled to a d-wave superconductor. When the coupling is asymmetric in real space, channel mixing arises in the Nambu space, and can lead to a transition from the doublet to the singlet ground state, even if it is missing in the absence of channel mixing. Our strategy applies to both Anderson and Kondo impurity models, and enables NRG solution of general channel-mixing quantum impurity models, as would be desirable in cluster dynamical mean field theory and dynamical cluster approximation.

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The Kondo impurity model and its associated Anderson impurity model are challenging many-body problems and play an important role in condensed matter physics.[1] Such models develop infrared logarithmic divergence in perturbation theory, and hence require nonperturbative solutions. The Kondo impurity model was first solved by Wilson using the simultaneously invented numerical renormalization group (NRG). [2] The NRG captures the physics at exponentially decreasing energy scales iteratively, a key ingredient behind its great success. It proves to be one of the most accurate and efficient methods for the quantum impurity problems, [3] and therefore has been broadly used as an impurity solver in the dynamical mean field theory (DMFT) and dynamical cluster approximation (DCA). [4–6]

The quantum impurity is coupled to a noninteracting conduction band (or bath), the effect of which is to cause a so-called hybridization function $\mathcal{D}(\omega)$. In the case of a scalar or diagonal matrix function $\mathcal{D}(\omega)$, a standard NRG procedure has been developed. [7–10] The key ingredient is to map the effect of $\mathcal{D}(\omega)$ into an open Wilson chain. As an interesting application, the NRG solution of the quantum impurity problem with a pseudogap bath that leads to $\mathcal{D}(\omega) \propto |\omega|^r$ reveals that for a particle-hole symmetric impurity the spin is always unscreened for $r > 1/2$.[7, 11] The $r = 1$ bath is of immediate experimental relevance since it is realized in nodal matters such as d-wave superconductor, neutral graphene and the surface of a topological insulator,[12–14], as long as the resulting $\mathcal{D}(\omega)$ is effectively spin independent.

However, the extension to quantum impurity models with $\mathcal{D}(\omega)$ non-diagonal in the spin and/or local orbital basis is not straightforward at all. Such a matrix function is said to be channel-mixing henceforth, with a channel referring to a combination of spin and orbital (as well as atomic site in a cluster). This situation naturally arises in the presence of spin-orbital coupling, Cooper pairing, as well as in a cluster impurity. The intertwining spin, charge and orbital degrees of freedom are promising for harvesting novel quantum effects, and the cluster impurity is invoked in DCA and cluster DMFT (cDMFT). These interesting and important cases are barely addressed by NRG in the literature so far because of the lack of a versatile scheme to map a channel-mixing $\mathcal{D}(\omega)$ to a Wilson chain. The only exception to our knowledge is the quantum impurity coupled locally to an s-wave superconductor with a particle-hole symmetric normal band.[15–18] However, the extension to more general cases is not yet available. We also notice that the channel-mixing model we will be addressing is different to the usual multi-channel model where $\mathcal{D}(\omega)$ is actually channel-diagonal, although the latter is interesting on its own right. [19]

In this Letter, we fill the gap caused by the above difficulties. We propose a versatile scheme to map a general (matrix) hybridization function into an open Wilson chain. We benchmark the mapping scheme against a nontrivial previous result,[15, 16] and we apply the scheme to investigate an Anderson impurity coupled to a d-wave superconductor. When the coupling is asymmetric in real space, channel mixing arises in the Nambu space, and is able to induce a quantum phase transition from the doublet to the singlet ground state, even if it is missing in the absence of channel mixing. [12] Our strategy enables NRG studies of general Anderson and Kondo impurities untouched before.

A versatile mapping scheme: For definiteness we consider a generalized Anderson impurity model, while the Kondo impurity model will be addressed in the closing section. The Hamiltonian $H = H_{imp} + H_b + H_{hyb}$ is composed of,

$$\begin{aligned} H_{imp} &= \sum_{\alpha,\beta} f^\dagger_\alpha h^{\alpha\beta}_{loc} f_\beta + H_{int}, \\ H_b &= \sum_{\mathbf{k},a,b} c^\dagger_{\mathbf{k},a} h^{ab}_{\mathbf{k}} c_{\mathbf{k},b}, \\ H_{hyb} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\alpha,a} (f^\dagger_\alpha \gamma^{\alpha a}_{\mathbf{k}} c_{\mathbf{k},a} + \text{h.c.}). \end{aligned} \tag{1}$$

Here f_α is an annihilation field at channel α of the impurity, $c_{\mathbf{k},a}$ an annihilation field at channel a and at momentum $\mathbf{k}$ in the bath, and N is the volume (or number of unit cells) in the bath. (The channel numbers in the impurity and the bath can differ in general.) As we mentioned, we take a channel index as a combined label of spin and orbital (as well as the site in a cluster impurity). The concrete expressions for the matrices h_{loc}, $h_{\mathbf{k}}$ and $\gamma_{\mathbf{k}}$, as well as the interaction H_{int} on the impurity are unnecessary at this stage.

Integrating out the free bath leads to a (matrix) self-energy correction to the impurity,

$$\Sigma(z) = \frac{1}{N} \sum_{\mathbf{k}} \gamma_{\mathbf{k}} G_{\mathbf{k}}(z) \gamma^\dagger_{\mathbf{k}}, \tag{2}$$

where $z = \omega \pm i0^+$ in the retarded/advanced case, and $G_{\mathbf{k}}(z) = 1/(z - h_{\mathbf{k}})$ is the Green's function at the complex frequency z. Via Kramers-Kronig relation, $\Sigma(z)$ can be completely characterized by

$$\mathcal{D}(\omega) = i[\Sigma(\omega + i0^+) - \Sigma(\omega - i0^+)]/2\pi. \tag{3}$$

which we call a (matrix) hybridization function. (For later convenience our definition differs to the usual one by a factor of π.) However, $\mathcal{D}(\omega)$ is in general non-diagonal, i.e., channel mixing. Our purpose is to map the effect of such a $\mathcal{D}(\omega)$ into that of a generalized open Wilson chain.

By definition, $\mathcal{D}(\omega)$ is hermitian and positive semi-definite. This enables us to write

$$\mathcal{D}(\omega) = \sum_n |n,\omega\rangle \rho_n(\omega) \langle n,\omega|, \tag{4}$$

where $\rho_n(\omega) \geq 0$ and $|n,\omega\rangle$ are the n-th eigenvalue and eigenvector of $\mathcal{D}(\omega)$. Similarly to the usual one-band case,[8, 9] we can re-express $\rho_n(\omega)$ as

$$\rho_n(\omega) = \int dx \; t^2_n(x) \delta[\omega - \epsilon_n(x)], \tag{5}$$

where $\epsilon_n(x)$ is a continuous function of x for each n, subject to the a requirement on the integration measures

$$t^2_n(x) dx = \rho_n[\epsilon_n(x)] \; |d\epsilon_n(x)|. \tag{6}$$

[The modulus symbol is necessary if $\epsilon_n(x)$ is a decreasing function of x.] The parametrization of $\epsilon_n(x)$ and $t_n(x)$ for $\rho_n(\omega)$ is similar to the usual logarithmic way,[3, 8, 9] and is also provided in the Supplementary Materials.

Substituting the expression of $\rho_n(\omega)$ into $\mathcal{D}(\omega)$, we write

$$\begin{aligned} \mathcal{D}(\omega) &= \int dx \; \sum_n |n,\omega\rangle t^2_n(x) \delta[\omega - \epsilon_n(x)] \langle n,\omega| \\ &= \int dx \; \sum_n |n,x\rangle t^2_n(x) \delta[\omega - \epsilon_n(x)] \langle n,x|, \end{aligned}$$

where we made a replacement $|n,\omega\rangle \to |n,x\rangle \equiv |n,\epsilon_n(x)\rangle$, valid in the presence of the delta-function in the integrand. This is a crucial step for the following discussions. In components, we have

$$\mathcal{D}_{\alpha\beta}(\omega) = \int dx \; \sum_n V_{\alpha n}(x) \delta[\omega - \epsilon_n(x)] V^\dagger_{n\beta}(x),$$

where $V_{\alpha n}(x) = t_n(x) \langle \alpha | n,x\rangle$. The above parametrization maps H_b and H_{hyb} to, respectively,

$$\begin{aligned} H'_b &= \int dx \sum_n \psi^\dagger_n(x) \epsilon_n(x) \psi_n(x), \\ H'_{hyb} &= \int dx \sum_{\alpha,n} f^\dagger_\alpha V_{\alpha n}(x) \psi_n(x) + \text{h.c.}, \end{aligned}$$

where ψ's are fermion fields in x. The mapping is exact since integrating out ψ's leads to the same $\Sigma(z)$ we started from. In practice, however, one would like to proceed in a discrete space of x. Fortunately, as in the usual case, the above mapping is designed such that its discretized version provides a good approximation. For example, one can take $x_j = (|j| + \eta)\text{sign}(j)$[8] with nonzero integer j and a real twisting factor $\eta \in (0, 1]$, and replace the integration over x to a summation over j. Each case of η represents an approximation of the continuum model, and as far as $\mathcal{D}(\omega)$ is concerned, the average over η reproduces exactly the result from the continuum model. A graphical representation of a discrete mapping is shown in Fig.1(a).

We proceed to map the discretized model to an open Wilson chain, a key ingredient of NRG to reduce the computational cost and optimize the scaling behavior. Let us assume the dimension of the single-particle Hilbert space of the impurity is I (the number of channels), and that for H'_b is $B = 2JI$, where J is the number of x_j's for $j > 0$ (or $j < 0$) retained in the discritization. Let us rewrite H'_b and H'_{hyb} compactly as

$$H'_b = \Psi^\dagger \mathcal{E} \Psi, \quad H'_{hyb} = F^\dagger \mathcal{V} \Psi + \Psi^\dagger \mathcal{V}^\dagger F,$$

where Ψ and F are spinors composed of the ψ- and f-fields, respectively. In this form, $\mathcal{E}_{B\times B}$ and $\mathcal{V}_{I\times B}$ are matrices, the dimensions of which are indicated by he subscripts. We perform a QR decomposition $\mathcal{V}^\dagger = U^\dagger_0 T^\dagger_0$, where $T^\dagger_0$ is an upper triangular matrix. We use the columns of $U^\dagger_0$ as the first set of Krylov basis vectors to transform $\mathcal{E}$, by block-Lanczos,[20, 21] into a block-tridiagonal matrix E_T (with block size I) such that

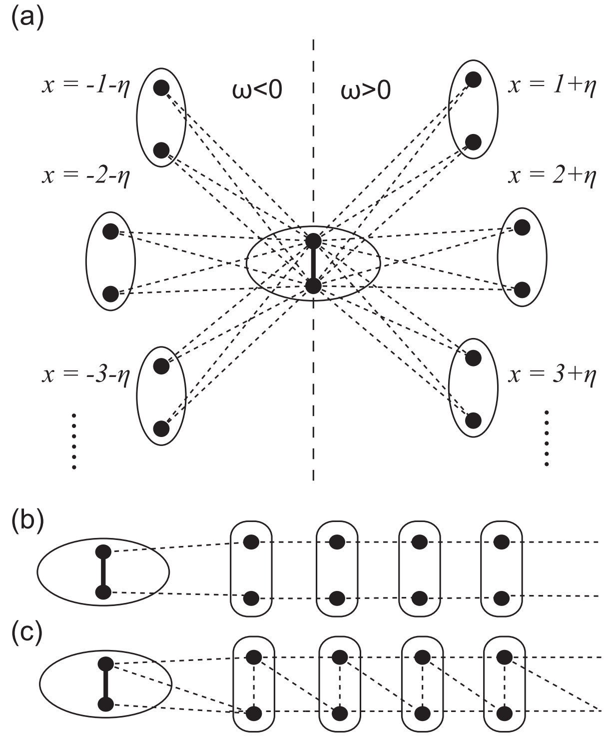

FIG. 1. Graphical illustrations of (a) the discretized bath coupled to the impurity, (b) a channel-diagonal Wilson chain in the usual case, and (c) a channel-mixing Wilson chain in general cases. The number of channels is set as (but not limited to) $I = 2$.

$\mathcal{E} = U^\dagger E_T U$, where the columns of $U^\dagger$ are Krylov basis vectors, and the leading ones are from $U_0^\dagger$. In the resulting Krylov space, or upon a canonical transformation $U\Psi \to \Phi$, we have

$$H'_b + H'_{hyb} \to \sum_{k=1}^{K} [\Phi_k^\dagger E_k \Phi_k + \Phi_{k-1}^\dagger T_{k-1} \Phi_k + \text{h.c.}], \quad (7)$$

where K is the number of block-Lanczos iterations, Φ_k denotes an I-component spinor such that $\Phi^\dagger = (\Phi_1^\dagger, \Phi_2^\dagger, \cdots, \Phi_K^\dagger)$, and we set $\Phi_0 = F$ for brevity. For $k \geq 1$, E_k (T_k) is the k-th $I \times I$ block element of E_T along the diagonal (upper sub-diagonal). Notice that all T_k's are triangular matrices themselves. Eq. (7) defines the open Wilson chain we were after. For comparison, the usual Wilson chain is illustrated in Fig.1(b), which is channel diagonal, while the Wilson chain in our general cases is illustrated in (c). In practice, the block-Lanczos procedure requires infinitely high precision and is truncated at a suitable stage $K \sim J$. Numerical examples of our mapping scheme for models discussed below can be found in the Supplementary Materials.

Comparison to a previous nontrivial case: Given the above versatile mapping, we are able to study a variety of new quantum impurity models, with or without channel mixing. Here we consider an Anderson impurity coupled to a conventional s-wave superconductor. The Hamiltonian in the Nambu space is composed of

$$H_{imp} = \psi_f^\dagger \epsilon_f \sigma_z \psi_f - \frac{1}{2} U (\psi_f^\dagger \sigma_z \psi_f)^2,$$
$$H_b = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger (\epsilon_{\mathbf{k}} \sigma_z + \Delta_{\mathbf{k}} \sigma_x) \psi_{\mathbf{k}},$$
$$H_{hyb} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \psi_f^\dagger t_{\mathbf{k}} \sigma_z \psi_{\mathbf{k}} + \text{h.c.}.$$

Here $\psi_f^\dagger = (f_\uparrow^\dagger, f_\downarrow)$ and $\psi_{\mathbf{k}}^\dagger = (c_{\mathbf{k}\uparrow}^\dagger, c_{-\mathbf{k}\downarrow})$ are Nambu spinors for the impurity and the bath, $\sigma_{x,z}$ are Pauli matrices in the Nambu space, ϵ_f is a measure of the deviation from particle-hole symmetry on the impurity, U is the Hubbard repulsion, $\Delta_{\mathbf{k}}$ is the pairing function of momentum $\mathbf{k}$ in the bath, and finally $t_{\mathbf{k}}$ is the momentum-dependent coupling amplitude between the impurity and the bath. We assume $\Delta_{\mathbf{k}} = \Delta$, $t_{\mathbf{k}} = t$ and $\epsilon_f = 0$ as in Ref.[15, 16]. We also assume a normal state band within the energy window $[-D_0, D_0]$ with a constant density of states $\rho_0 = 1/2D_0$. Henceforth we take $D_0 = 1$ as the unit of energy. Integrating out the superconducting bath, we get $\Sigma(z)$ and subsequently

$$\mathcal{D}(\omega) = \frac{\Gamma(\omega\sigma_0 - \Delta\sigma_x)\text{sign}(\omega)}{\pi\sqrt{\omega^2 - \Delta^2}} W(\omega^2 - \Delta^2),$$

where $\Gamma = \pi\rho_0 t^2$ and σ_0 is the 2×2 identity matrix. Henceforth $W(u) = \theta(u)\theta(1-u)$ is a window function.

We map the system to a Wilson chain as described above, and we perform NRG iterations thereafter. The iteration converges quickly, and we monitor the energy E of the lowest excited state on top of the many-body ground state as a function of U. The results are shown in Fig.2 for $\Delta = 0.01$ (gray solid line) and $\Delta = 0.1$ (black solid line). The NRG results in the free limit $U = 0$ is in

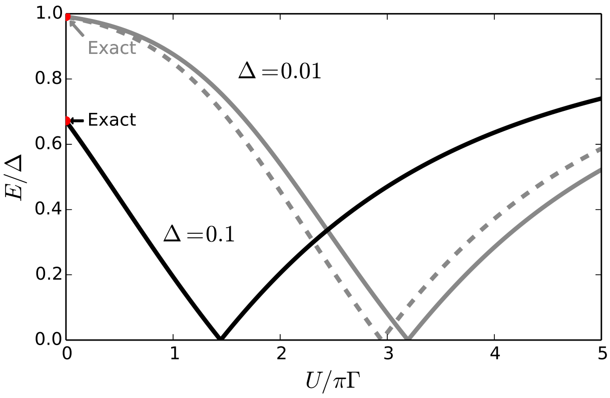

FIG. 2. The first excitation energy E as a function of U for $\Delta = 0.01$ (gray solid line) and $\Delta = 0.1$ (black solid line). The dashed line is the result for $\Delta = 0.01$ but with proper accounting of the under-estimation in Ref.[16] for comparison. See the text for details.

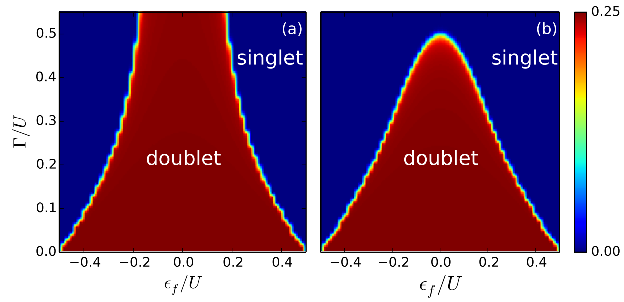

FIG. 3. The phase diagram for (a) $t_2 = 0$ and (b) $t_2 = 0.1$. The color indicates the magnitude of M^2. At zero temperature, the phase boundary would be sharp and mark the transition from doublet to singlet ground states.

excellent agreement with the analytical results (arrows) from the Green's function method. With increasing U, we see, in either case of Δ, a cusp at which $E = 0$. It is known that this corresponds to a singlet-doublet transition of the many-body ground state. Our transition point for $\Delta = 0.01$ (gray solid line) is slightly larger than that in Ref.[16]. This is however not an inconsistency. In fact, the discretization scheme in Ref.[16] under-estimates the effect of Γ by a factor of $A = \frac{1}{2}\frac{\Lambda+1}{\Lambda-1}\ln\Lambda$, [3, 8] where Λ is a scaling factor. For $\Lambda = 2.5$ used in Ref.[16], $A \sim 1.069$. Thus for a fair comparison, we use $\Gamma' = \Gamma/A$ in our calculation, and present the data at Γ instead. The result is shown as the dashed line in Fig.2, which is now in agreement with that in Ref.[16].

Application to an intriguing case: We now consider a d-wave superconducting bath. We use the same normal band as before. In case of constant $t_{\mathbf{k}}$, $\mathcal{D}(\omega)$ is actually diagonal, the effect of which is equivalent to that of a nodal normal metal that can not screen the impurity spin at $\epsilon_f = 0$.[16] In this respect, it is interesting to ask how an off-diagonal (channel-mixing) term in $\mathcal{D}(\omega)$ would occur and how it would affect the fate of impurity spin at zero temperature. This is an issue not yet addressed.

In fact, to induce channel-mixing in our case, all that we need is a $t_{\mathbf{k}}$ asymmetric under the point group. For example, in a lattice model of the bath, if the impurity is coupled, via hopping integral t, only to two sites at $\mathbf{r} = \pm\hat{x}/2$ on a nearest-neighbor bond, we would have $t_{\mathbf{k}} = 2t\cos(k_x/2)$ (in a suitable gauge). This can be resolved into A_{1g} and B_{1g} lattice harmonics. Thus in general, we may assume $t_{\mathbf{k}} \to t_\phi = \sum_l t_l e^{il\phi}$ in the continuum limit, with ϕ the azimuthal angle of $\mathbf{k}$, and $t_{-l} = t_l^*$ required by time-reversal symmetry. In the same limit we write $\Delta_{\mathbf{k}} \to \Delta_\phi = \Delta\cos(2\phi)$. For concreteness, we assume $t_\phi = t_0 + 2t_2\cos(2\phi)$, and we fix $t_0 = 1$ and $\Delta = 0.1$ in the calculations.

The d-wave superconducting bath leads to

$$\mathcal{D}(\omega) = \int \frac{d\phi}{2\pi} \frac{\Gamma|t_\phi|^2(\omega\sigma_0 - \Delta_\phi\sigma_x)\mathrm{sign}(\omega)}{\pi|t_0|^2\sqrt{\omega^2 - \Delta_\phi^2}} W(\omega^2 - \Delta_\phi^2),$$

where $\Gamma = \pi\rho_0 t_0^2$. We make the resolution $\mathcal{D}(\omega) = d_0(\omega)\sigma_0 + d_x(\omega)\sigma_x$ to find, for $|\omega| \ll 1$, $d_0(\omega) \sim (t_0^2 + 2t_2^2)|\omega|/\Delta$ and $d_x(\omega) \sim t_0 t_2\omega|\omega|/\Delta^2$. Thus t_2 leads to a channel-mixing component $d_x(\omega)$. We map the model to an open Wilson chain as described above, and perform NRG investigations thereafter. We consider the static magnetic susceptibility $\chi_{\mathrm{imp}}(T) = \chi_{\mathrm{tot}}(T) - \chi_{\mathrm{tot}}^{(0)}(T)$ at an energy scale $T \sim 10^{-6}D$ (the zero temperature limit).[3] Here, χ_{tot} ($\chi_{\mathrm{tot}}^{(0)}$) is the total susceptibility calculated with (without) the impurity. An effective moment scale M can be defined by $M^2 = T\chi_{imp}(T)$. One expects M^2 to vanish if the impurity spin is screened, while $M^2 = 1/4$ if a full local moment survives. In fact, they correspond to the singlet and doublet ground states, respectively. Fig.3 shows M^2 (color scale) as a function of ϵ_f/U and Γ/U, with $\pi\Gamma = 0.5$ fixed, for the two typical cases $t_2 = 0$ (a) and $t_2 = 0.1$ (b). In both cases there appears a transition from $M^2 = 1/4$ to $M^2 = 0$ with increasing Γ/U for a large $|\epsilon_f|/U$. However, there is a marked difference when $\epsilon_f = 0$, the particle-hole symmetric point for the impurity: while a full local moment persists for $t_2 = 0$ in (a), we do find a transition from the local moment phase to complete screening as Γ/U increases for $t_2 = 0.1$ in (b). Thus $d_x(\omega)$ plays an essential role here. It would be interesting to see whether a hypothetical $d_x(\omega) \sim |\omega|^\kappa \mathrm{sign}(\omega)$ would fail to screen the impurity spin for other cases of exponent κ, which we leave in a future work.

Summary and remarks: We developed a versatile scheme to map a general quantum impurity model to an open Wilson chain, resolving the difficulty caused by channel mixing. This fills the gap *hitherto* toward NRG studies of impurity models with spin-orbital coupling, Cooper pairing and/or cluster impurity, as would be desirable in DCA and cDMFT. After the comparison to a nontrivial previous result, we apply the scheme for an Anderson impurity coupled to a d-wave superconductor. We found that an asymmetric coupling leads to channel-mixing in the Nambu space and can lead to a transition from the doublet to the singlet ground state that would be missing in the absence of channel mixing.

We remark how our mapping scheme also applies to general Kondo impurity models. Suppose the bath is composed of two parts A and B, and only A is coupled via spin-exchange to the quantum impurity I. The idea is to map the effect of B on A as an open Wilson chain C that starts from A. Then $I \otimes C$ forms the suitable system for NRG iterations. A mapping scheme exists for a Kondo impurity coupled locally to an s-wave supercondcutor,[18] however the extension is not yet available for more general cases of pairing, spin-orbital coupling and/or nonlocal coupling to the bath.

There is no difficulty in our strategy instead.

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