Supplementary Materials: Analogue Black Holes in Reactive Molecules

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Text A: Hawking radiation and IHO

In this section, we show that the equation of motion of a scalar field near the event horizon of Schwarzschild black hole (BH) is of the same form as the stationary Schrödinger equation of the inverted harmonic oscillator (IHO). Near the event horizon, the Schwarzschild metric can be reduced to the Rindler metric which describes the spacetime of a uniformly accelerating system. To this end, we define

$$\rho = \int_{r_s}^{r} \left(1 - \frac{r_s}{r'}\right)^{-1/2} dr' = \sqrt{r(r - r_s)} + r_s \tanh^{-1}\left(\sqrt{1 - \frac{r_s}{r}}\right). \tag{S1}$$

Near the event horizon, ρ can be approximated by

$$\rho \approx 2\sqrt{r_s(r - r_s)}, \tag{S2}$$

and the Schwarzschild metric can be written as

$$ds^2 \approx \rho^2 \left(\frac{cdt}{2r_s}\right)^2 - d\rho^2 - \left(\frac{\rho^2}{4r_s} + r_s\right)^2 (d\theta^2 + \sin^2\theta d\varphi^2). \tag{S3}$$

Due to the rotational symmetry, we could only consider the radial part. By defining a dimensionless time $\tau = ct/(2r_s)$, we have the Rindler metric in the $1+1$ spacetime,

$$ds^2 = \rho^2 d\tau^2 - d\rho^2, \tag{S4}$$

which can also be written into a conformally flat form by choosing a new spatial coordinate $\xi = \kappa^{-1}\ln(\kappa\rho)$ and rescaling $\tau \to \tau/\kappa$. Then we have the following metric

$$ds^2 = e^{2\kappa\xi}(d\tau^2 - d\xi^2). \tag{S5}$$

Then equation of motion of scalar field near the event horizon can be written as

$$\left(\frac{\partial^2}{\partial\tau^2} - \frac{\partial^2}{\partial\xi^2}\right)\phi(\tau,\xi) = 0. \tag{S6}$$

The eigen modes are

$$\phi_\pm(\tau,\xi) = e^{\pm i\Omega(\xi\mp\tau)}, \tag{S7}$$

which satisfy $i\partial_\tau\phi_\pm = \Omega\phi_\pm$ and can be understood as the right/left-moving modes. If we define

$$u = -\frac{e^{\kappa(\xi-\tau)}}{\kappa}; \quad v = \frac{e^{\kappa(\xi+\tau)}}{\kappa}, \tag{S8}$$

and the scaling operators

$$\hat{\mathcal{S}}_v = -iv\partial_v; \quad \hat{\mathcal{S}}_u = iu\partial_u, \tag{S9}$$

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Eq.(S6) becomes

$$\hat{\mathcal{S}}_u\hat{\mathcal{S}}_v\phi(u,v)=0. \tag{S10}$$

Noticing that $\partial_\tau = i\kappa(\hat{\mathcal{S}}_u+\hat{\mathcal{S}}_v)$, the two independent solutions $\phi_1(u,v)\equiv\phi_1(u)$ and $\phi_2(u,v)\equiv\phi_2(v)$ thus satisfy

$$\hat{\mathcal{S}}_u\phi_1(u)=-\frac{\Omega}{\kappa}\phi_1(u);\quad \hat{\mathcal{S}}_v\phi_2(v)=-\frac{\Omega}{\kappa}\phi_2(v), \tag{S11}$$

and

$$\phi_1(u,v)=(-\kappa u)^{i\Omega/\kappa},\quad \phi_2(u,v)=(\kappa v)^{-i\Omega/\kappa}, \tag{S12}$$

which can also be obtained from Eq.(S7) using Eq.(S8). Eq. (S12) as eigenfunctions of ∂_τ and the scaling operators $\hat{\mathcal{S}}_{u/v}$ underlie the Hawking-Unruh radiation [1, 2].

On the other hand, The Hamiltonian of the inverted harmonic oscillator is written as

$$\hat{H}_{\text{IHO}}=\frac{\hat{p}^2}{2m}-\frac{1}{2}m\omega^2\hat{x}^2. \tag{S13}$$

We define a new set of variables

$$\hat{u}^{\pm}=\frac{\hat{p}\pm m\omega\hat{x}}{\sqrt{2m\omega}}, \tag{S14}$$

and it can be check that $[\hat{u}^+,\hat{u}^-]=i\hbar$. Then, the IHO Hamiltonian can be rewritten as

$$\hat{H}_{\text{IHO}}=\frac{\omega}{2}\left(\hat{u}^+\hat{u}^-+\hat{u}^-\hat{u}^+\right). \tag{S15}$$

Now we consider the solutions to the Schrödinger equation in two distinct representations:

- In the u^+-space, we have

$$\hat{H}_{\text{IHO}}=\frac{\omega}{2}\left(2\hat{u}^+\hat{u}^- - i\hbar\right)=-i\hbar\omega\left(u^+\partial_{u^+}+\frac{1}{2}\right), \tag{S16}$$

  and the solution to the Schrödinger equation $\hat{H}_{\text{IHO}}\psi(u^+)=E\psi(u^+)$ reads $\psi(u^+)=(\pm u^+)^{\frac{iE}{\hbar\omega}-\frac{1}{2}}$.

- In the u^--space, we have

$$\hat{H}_{\text{IHO}}=\frac{\omega}{2}\left(2\hat{u}^-\hat{u}^+ + i\hbar\right)=i\hbar\omega\left(u^-\partial_{u^-}+\frac{1}{2}\right), \tag{S17}$$

  and the solution to the Schrödinger equation $\hat{H}_{\text{IHO}}\psi(u^-)=E\psi(u^-)$ reads $\psi(u^+)=(\pm u^-)^{-\frac{iE}{\hbar\omega}-\frac{1}{2}}$.

Comparing Eq.(S11) with Eq.(S16), (S17), we find that near the event horizon, the dynamic of a scalar field, up to a constant energy shift, can be reduced to that of IHO.

Text B: Imperfect event horizon

The reflection and transmission with a generic "quantum defect" parameter y can be obtained by studying multiple scatterings between an imperfect event horizon and potential barrier, as shown in Fig. S1. The imperfect event horizon partially reflects the incoming waves and thus corresponds to a reaction rate less than unity. According to the quantum defect theory (QDT), the short range asymptotic behavior of the radial wave function is written as

$$u_\ell(r\to 0)\propto\frac{r^{3/2}}{\beta_6}\left[e^{i\left(\frac{1}{2}\left(\frac{\beta_6}{r}\right)^2-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right)}-\frac{1-\frac{1}{iK_\ell^0}}{1+\frac{1}{iK_\ell^0}}e^{-i\left(\frac{1}{2}\left(\frac{\beta_6}{r}\right)^2-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right)}\right] \tag{S18}$$

where K_ℓ^0 is the ℓ-th wave K-matrix [3]. We define the "quantum-defect" parameter y in the following way

$$\frac{1-\frac{1}{iK_\ell^0}}{1+\frac{1}{iK_\ell^0}}=\frac{1-y}{1+y}e^{-2i\eta_\ell}, \tag{S19}$$

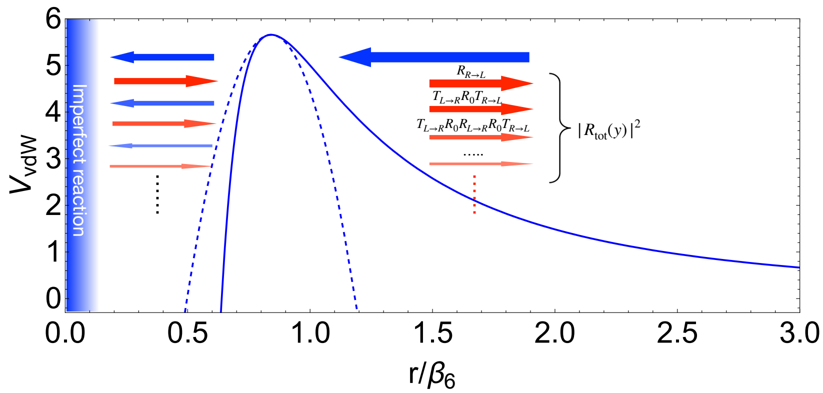

FIG. S1. A schematic of multiple scatterings caused by an imperfect event horizon. $R_{R(L)\to L(R)}$ and $T_{R(L)\to L(R)}$ indicate the reflection and transmission amplitude for the "right(left) to left(right)" scattering. $R_{\rm tot}(y)$ denotes the total reflection amplitude with generic "quantum parameter" y. It can be obtained by summing over such an infinite series of scatterings. Blue and red arrows denote the left and right moving waves. The solid and dashed curves depict the interaction between two molecules with high partial-wave scatterings (or dipole-dipole interactions) and the IHO approximation, respectively.

where η_ℓ is the scattering phase shift. For the case that $y = 1$, $K^0_\ell = -i$, and the second term in Eq.(S18) vanishes, which corresponds to complete absorption. For the case that $y = 0$, $K_\ell = -\frac{1}{\tan\eta_\ell}$, which corresponds to a complete reflection, i.e., a perfect event horizon. For the generic case, the K-matrix is y-dependent via,

$$K^0_\ell(y) = -\frac{1}{\tan\eta_\ell} + y\frac{1+\tan^2\eta_\ell}{(y+i\tan\eta_\ell)\tan\eta_\ell}. \tag{S20}$$

The long-range asymptotic behavior of the radial wave function is written as

$$\begin{aligned} u_\ell(r\to\infty) \propto & \left(K^0_\ell(y)Z_{gg} - Z_{fg} + i\left(K^0_\ell(y)Z_{gf} - Z_{ff}\right)\right)e^{i\left(kr-\frac{\ell\pi}{2}\right)} \\ & + \left(K^0_\ell(y)Z_{gg} - Z_{fg} - i\left(K^0_\ell(y)Z_{gf} - Z_{ff}\right)\right)e^{-i\left(kr-\frac{\ell\pi}{2}\right)}, \end{aligned} \tag{S21}$$

where $Z_{gg}, Z_{gf}, Z_{fg}, Z_{ff}$ are the element of the Z-matrix which is defined in Ref. [3]. Then we find the reflection amplitude is written as

$$R(y) = \frac{K^0_\ell(y)Z_{gg} - Z_{fg} + i\left(K^0_\ell(y)Z_{gf} - Z_{ff}\right)}{K^0_\ell(y)Z_{gg} - Z_{fg} - i\left(K^0_\ell(y)Z_{gf} - Z_{ff}\right)}. \tag{S22}$$

We would like to point out that this result can be explained by taking into account an infinite series of bounces between the potential barrier and the imperfect event horizon. To this end, we distinguish the "right-to-left scattering" and "left-to-right scattering" through the potential barrier.

- Right to left scattering; In such case, the short range boundary condition is written as

$$u_{R\to L}(r\to 0) \propto \frac{r^{3/2}}{\beta_6}e^{i\left[\frac{1}{2}\left(\frac{\beta_6}{r}\right)^2 - \frac{\nu_0\pi}{2} - \frac{\pi}{4}\right]} \tag{S23}$$

  which means $K^0_\ell = -i$, and then we have

$$u_{R\to L}(r\to\infty) \propto \left[\left(Z_{gf} - Z_{fg} - iZ_{ff} - iZ_{gg}\right)e^{i\left(kr-\frac{\ell\pi}{2}\right)} + \left(iZ_{ff} - iZ_{gg} - Z_{gf} - Z_{fg}\right)e^{-i\left(kr-\frac{\ell\pi}{2}\right)}\right], \tag{S24}$$

  and the corresponding reflection and transmission amplitude are

$$R_{R\to L} = \frac{Z_{gf} - Z_{fg} - i(Z_{ff} + Z_{gg})}{i(Z_{ff} - Z_{gg}) - (Z_{fg} + Z_{gf})}; \quad T_{R\to L} = \frac{2\sqrt{2}}{i(Z_{ff} - Z_{gg}) - (Z_{gf} + Z_{fg})}, \tag{S25}$$

  respectively. Using the fact that $Z_{ff}Z_{gg} - Z_{fg}Z_{gf} = -2$, it is readily to verify $|R_{R\to L}|^2 + |T_{R\to L}|^2 = 1$.

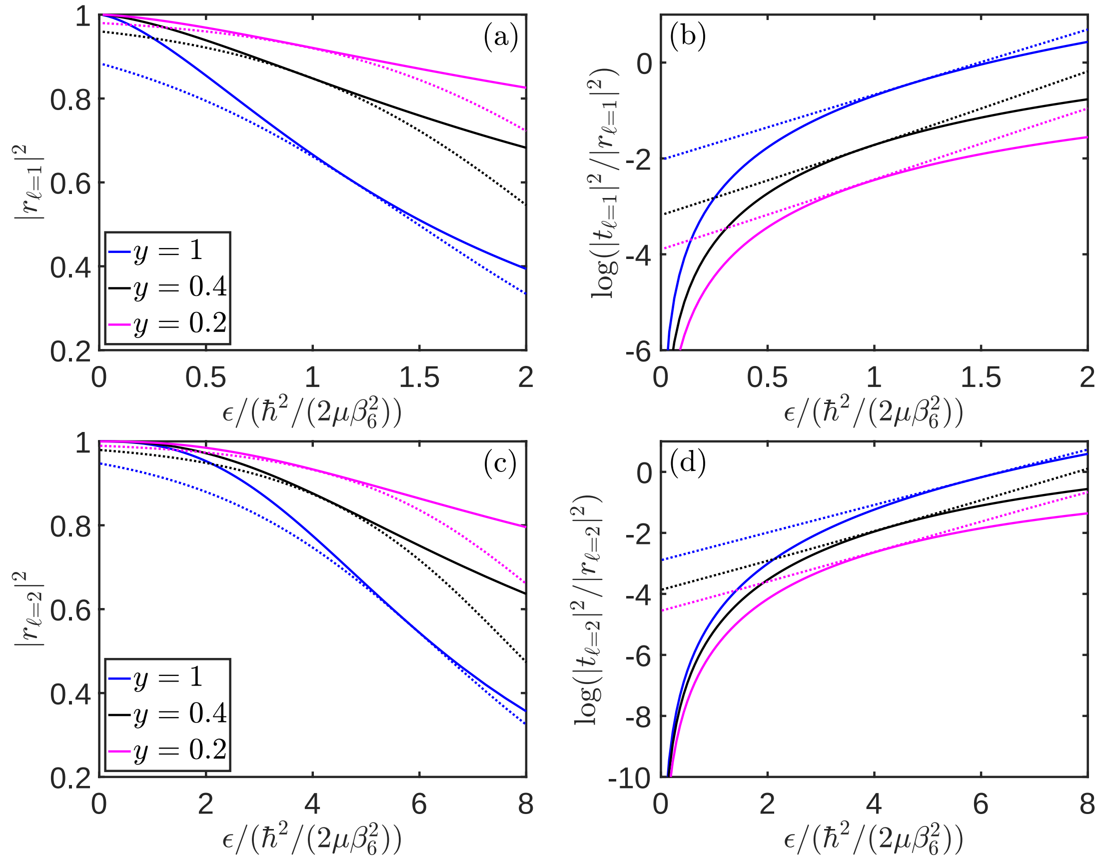

FIG. S2. Reflection rate $|r_\ell|^2$ and $\log\left(|t_\ell|^2/|r_\ell|^2\right)$ of reactive molecule under imperfect absorbing boundary condition for p-wave (a,b) and d-wave (c,d) scattering.The solid curves depict the results of van der Waals potential and the dashed curves show the results of IHO.

- Left to right scattering; In such case, the long range boundary condition is written as

$$u_{L\to R}(r\to\infty)\propto\left(\left(K_\ell^0 Z_{gg}-Z_{fg}\right)+i\left(K_\ell^0 Z_{gf}-Z_{ff}\right)\right)e^{i\left(kr-\frac{\ell\pi}{2}\right)} + \left(\left(K_\ell^0 Z_{gg}-Z_{fg}\right)-i\left(K_\ell^0 Z_{gf}-Z_{ff}\right)\right)e^{-i\left(kr-\frac{\ell\pi}{2}\right)}. \tag{S26}$$

Since the second term is required to vanish, we have

$$\left(K_\ell^0 Z_{gg}-Z_{fg}\right)-i\left(K_\ell^0 Z_{gf}-Z_{ff}\right)=0, \tag{S27}$$

i.e.,

$$K_\ell^0=\frac{Z_{fg}-iZ_{ff}}{Z_{gg}-iZ_{gf}}. \tag{S28}$$

Then the short range boundary condition can be written as

$$u_{L\to R}(r\to 0)\propto\frac{r^{3/2}}{\beta_6}\left[\frac{Z_{gg}+Z_{ff}+i(Z_{fg}-Z_{gf})}{Z_{gg}-iZ_{gf}}e^{i\left(\frac{1}{2}\left(\frac{\beta_6}{r}\right)^2-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right)} + \frac{Z_{gg}-Z_{ff}-i(Z_{fg}+Z_{gf})}{Z_{gg}-iZ_{gf}}e^{-i\left(\frac{1}{2}\left(\frac{\beta_6}{r}\right)^2-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right)}\right], \tag{S29}$$

and the corresponding reflection and transmission amplitude are written as

$$R_{L\to R}=\frac{(Z_{fg}-Z_{gf})-i(Z_{gg}+Z_{ff})}{i(Z_{ff}-Z_{gg})-(Z_{fg}+Z_{gf})};\quad T_{L\to R}=\frac{\sqrt{2}(Z_{fg}Z_{gf}-Z_{ff}Z_{gg})}{i(Z_{ff}-Z_{gg})-(Z_{fg}+Z_{gf})}, \tag{S30}$$

respectively. It can also be checked that $|R_{L\to R}|^2+|T_{L\to R}|^2=1$.

We use $R_0=-\frac{1-y}{1+y}e^{2i\eta_\ell}$ to characterize the reflection amplitude near the event horizon, where η_ℓ is the phase shift of the elastic scattering. Then the total reflection amplitude can be written as

$$\begin{aligned} R_{\mathrm{tot}}(y) =& R_{R\to L}+T_{L\to R}R_0T_{R\to L}+T_{L\to R}R_0R_{L\to R}R_0T_{R\to L}+T_{L\to R}R_0R_{L\to R}R_0R_{L\to R}R_0T_{R\to L}+...\\ =& R_{R\to L}+T_{L\to R}\frac{R_0}{1-R_0R_{L\to R}}T_{R\to L}. \end{aligned} \tag{S31}$$

By substituting Eq.(S25) and Eq.(S30) into Eq.(S31), we immediately find $R_{\mathrm{tot}}(y)=R(y)$. As a result, the thermal-like tunneling can be extracted from the decay rate of any y.

In the same spirit, we can obtain the scattering amplitude of IHO by implementing an imperfect absorbing boundary condition at the imperfect event horizon. Considering the reflection symmetry of the IHO potential, we have

$$|r_{\mathrm{IHO}}|^2(y)=\left|\frac{R-R_0(R^2-T^2)}{1-R_0R}\right|^2, \tag{S32}$$

where $R=S_{11}$ and $T=S_{12}$ are the reflection and transmission amplitude of IHO, as shown in Eq.(5) of the main text. In Fig. S2, we show the reflection rate of van der Waals potential under the partial absorbing boundary condition provided by an imperfect event horizon. It is clear that the IHO provides a good approximation for a generic y.

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