Supplemental material: Five-body Efimov effect and universal pentamer in Fermionic mixtures

DIFFUSION METHOD FOR SOLVING THE STM EQUATION

In this section we describe the diffusion process in detail in the case $N = 4$ (pentamer), the other cases being treated in the same manner. We write

$$F(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = g(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) f(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3), \tag{S1}$$

and choose g in the form

$$g(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = \frac{\mathbf{q}_1 \cdot \mathbf{q}_2 \times \mathbf{q}_3}{|\mathbf{q}_1 \cdot \mathbf{q}_2 \times \mathbf{q}_3|} \frac{4\pi(q_1^2 + q_2^2 + q_3^2)^{\frac{\alpha}{2}} q_1^\beta q_2^\beta q_3^\beta}{\kappa_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} - \frac{1}{a} - \frac{r_0}{2}\kappa^2_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}}, \tag{S2}$$

where $\kappa^2_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} = -\frac{2\mu E}{\hbar^2} + \frac{\mu}{M}(q_1^2 + q_2^2 + q_3^2) + \frac{\mu}{M+m}(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3)^2$ and α and β are parameters, the choice of which is discussed below.

The function $f(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)$ in Eq. (S1) is symmetric with respect to permutations of $\mathbf{q}_i$ and $\mathbf{q}_j$. Moreover, it can be written in the form

$$f(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = f(q_1, q_2, q_3, \mathbf{q}_2 \cdot \mathbf{q}_3, \mathbf{q}_3 \cdot \mathbf{q}_1, \mathbf{q}_1 \cdot \mathbf{q}_2), \tag{S3}$$

which, in particular, means that

$$f(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = f(\tilde{\mathbf{q}}_1, \mathbf{q}_2, \mathbf{q}_3), \tag{S4}$$

where by $\tilde{\mathbf{q}}_i$ we denote the mirror image of $\mathbf{q}_i$ with respect to the plane spanned by $\mathbf{q}_j$ and $\mathbf{q}_k$ ($\{i, j, k\}$ are cyclic permutations of $\{1, 2, 3\}$). Explicitly, $\tilde{\mathbf{q}}_i = \mathbf{q}_i - 2(\mathbf{q}_i \cdot \hat{\mathbf{n}}_i)\hat{\mathbf{n}}_i$, where $\hat{\mathbf{n}}_i = \mathbf{q}_j \times \mathbf{q}_k / |\mathbf{q}_j \times \mathbf{q}_k|$. Note that κ and f are symmetric and g – antisymmetric with respect to $\mathbf{q}_i \to \tilde{\mathbf{q}}_i$.

Our diffusion process is based on the following. Consider a nine-dimensional element $d^3q_1 d^3q_2 d^3q_3$ placed at $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3$ and define the distribution function

$$P_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q}) = -\frac{\mathbf{q} \cdot \mathbf{q}_2 \times \mathbf{q}_3}{|\mathbf{q} \cdot \mathbf{q}_2 \times \mathbf{q}_3|} \frac{g(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)}{8\pi^3(q^2 + q_2^2 + q_3^2)^{\frac{\alpha}{2}} q^\beta q_2^\beta q_3^\beta} \left\{ \frac{1}{\kappa^2_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} + [\mathbf{q} + \mu(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3)/m]^2} - (\mathbf{q}_1 \to \tilde{\mathbf{q}}_1) \right\}, \tag{S5}$$

which is nowhere negative, and introduce the corresponding normalization integral

$$W_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} = \int d^3q P_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q}). \tag{S6}$$

Assuming that we start with dN_w walkers in $d^3q_1 d^3q_2 d^3q_3$ we create three groups of new walkers with populations $dN_w W_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}$, $dN_w W_{\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_1}$ and $dN_w W_{\mathbf{q}_3,\mathbf{q}_1,\mathbf{q}_2}$, respectively. Then for each walker in group i we randomly move $\mathbf{q}_i$ to $\mathbf{q}$ keeping $\mathbf{q}_j$ and $\mathbf{q}_k$ unchanged. Here $\mathbf{q}$ is drawn from the normalized probability density distribution $P_{\mathbf{q}_i,\mathbf{q}_j,\mathbf{q}_k}(\mathbf{q})/W_{\mathbf{q}_i,\mathbf{q}_j,\mathbf{q}_k}$. As a result we obtain $dN_w(W_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} + W_{\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_1} + W_{\mathbf{q}_3,\mathbf{q}_1,\mathbf{q}_2})$ walkers distributed such that only one of their momenta is different from the initial one.

Let us now assume that walkers are initially distributed over the whole space according to the probability density distribution $f(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)$ and consider one such diffusive iteration acting simultaneously over all space elements. Then, the change in the density of walkers equals

$$\delta f(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = -f(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) + \int d^3q [P_{\mathbf{q},\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q}_1) f(\mathbf{q}, \mathbf{q}_2, \mathbf{q}_3) + P_{\mathbf{q}_1,\mathbf{q},\mathbf{q}_3}(\mathbf{q}_2) f(\mathbf{q}_1, \mathbf{q}, \mathbf{q}_3) + P_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}}(\mathbf{q}_3) f(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q})]. \tag{S7}$$

The direct substitution of Eqs. (S1), (S2), and (S5) into Eq. (S7) shows that the equilibrium condition $\delta f(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = 0$ leads to the STM Eq. (1) of the main text.

We model this diffusion process by using a finite number of walkers $N_w^{(i)}$ (i stands for the iteration number), which we keep close to an initially chosen average number N_w. For each walker with coordinates $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3$ we create $\lfloor W_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} \rfloor$ copies plus another one with probability $W_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} - \lfloor W_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} \rfloor$, where $\lfloor W \rfloor$ denotes the integer part of W. This gives on average $W_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}$ copies, the first momentum of which we move to different $\mathbf{q}$ drawn from $P_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q})/W_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}$. We do the same with the other two momenta.

The total population of walkers, apart from the statistical noise due to the above branching procedure, can be controlled by tuning one of the parameters E, a,

r_0, or M/m. We typically tune a at fixed E, r_0, and M/m. In each iteration we sum $\partial(W_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}+W_{\mathbf{q}_2,\mathbf{q}_3,\mathbf{q}_1}+W_{\mathbf{q}_3,\mathbf{q}_1,\mathbf{q}_2})/\partial a$ over the walkers and use it to estimate how strongly we need to change a in order to have $N_w^{(i+1)}$ close to N_w. We thus have a sequence of $a^{(i)}$ which fluctuates around an average value. The amplitude of these fluctuations decreases with N_w and $a^{(i)}$ averaged over many iterations converges to the exact a in the limit $N_w \to \infty$.

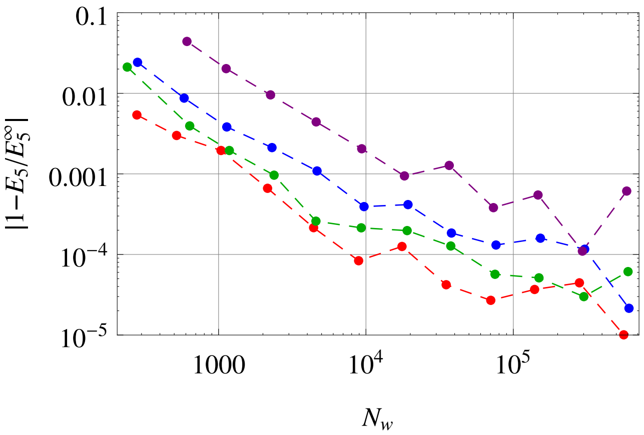

FIG. S1: The convergence of the pentamer energy E_5 towards E_5^∞ (assumed exact value in the limit $N_w \to \infty$) with increasing the number of walkers N_w for various M/m, from bottom to top: 10 (red), 11 (green), 12 (blue) and 13 (purple).

In Fig. S1 we show our analysis of the convergence of the pentamer energy with increasing N_w for $M/m = 10$ (red), 11 (green), 12 (blue) and 13 (purple). For these data we use $\alpha = 0$ and $\beta = 2$.

SAMPLING AND NORMALIZATION

In this section we outline the sampling procedure for the distribution function (S5) and calculation of the normalization integral (S6). First note that

$$P_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q}) = P_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\tilde{\mathbf{q}}) = P_{\tilde{\mathbf{q}}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q}). \tag{S8}$$

Therefore, we can restrict ourselves to the domain $\mathbf{q}_1 \cdot \mathbf{q}_2 \times \mathbf{q}_3 > 0$ and sample only in the domain $\mathbf{q}\cdot\mathbf{q}_2\times\mathbf{q}_3 > 0$. We then introduce the reduced distribution function

$$P^{\text{reduced}}_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q}) = \frac{g(\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3)}{8\pi^3 q_2^\beta q_3^\beta} \frac{(q^2+q_2^2+q_3^2)^{-\frac{\alpha}{2}} q^{-\beta}}{\kappa^2_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3} + (\mathbf{q}+\mathbf{v})^2}, \tag{S9}$$

where $\mathbf{v} = \mu(\tilde{\mathbf{q}}_1 + \mathbf{q}_2 + \mathbf{q}_3)/m$. The distribution function (S9) is, in the chosen domain, larger than $P_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q}) = P^{\text{reduced}}_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q}) - P^{\text{reduced}}_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\tilde{\mathbf{q}})$. Thus, in order to sample $P_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q})$ we use the rejection technique. Namely, we draw $\mathbf{q}$ from (S9) and accept it with the probability $P/P^{\text{reduced}} < 1$. The sampling of (S9) is realized by using spherical coordinates in which the zenith direction is along $\mathbf{v}$. Sampling the angles is trivial and the radial coordinate q is distributed according to

$$P(q)dq \propto \frac{q^{1-\beta}}{(q^2+q_2^2+q_3^2)^{\frac{\alpha}{2}}} \ln\frac{\kappa^2+v^2+q^2+2vq}{\kappa^2+v^2+q^2-2vq} dq, \tag{S10}$$

which we sample by using again the rejection method. In particular, in the case $\alpha > 2-\beta$ we use the proposal distribution $\propto dq/(\kappa^2+v^2+q^2)$ and the rejection algorithm then relies on the inequality

$$\frac{1}{q}\ln\frac{\kappa^2+v^2+q^2+2vq}{\kappa^2+v^2+q^2-2vq} \le \frac{2\sqrt{\kappa^2+v^2}}{\kappa^2+v^2+q^2}\ln\frac{\sqrt{\kappa^2+v^2}+v}{\sqrt{\kappa^2+v^2}-v} \tag{S11}$$

and on the fact that $q^{2-\beta}(q^2+q_2^2+q_3^2)^{-\frac{\alpha}{2}}$ is bounded from above. We find that this method works well for all parameters (κ, v, q_2, q_3, α, β) that we typically deal with.

The normalization integral (S6) is equivalent to integrating $P^{\text{reduced}}_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\mathbf{q}) - P^{\text{reduced}}_{\mathbf{q}_1,\mathbf{q}_2,\mathbf{q}_3}(\tilde{\mathbf{q}})$ over the half space $\mathbf{q}\cdot\mathbf{q}_2\times\mathbf{q}_3 > 0$. We find it convenient to perform this integration in spherical coordinates with the zenith direction along $\mathbf{q}_2\times\mathbf{q}_3$. The angular integrals are analytic and we end up with a one-dimensional integral over q which is numerically fast.

CHOICE OF α AND β

An obvious constraint on possible values of α and β is the convergence of the normalization integral (S6). In practice, as we have explained, we require $\alpha > 2-\beta$ for sampling convenience. In fact, we find that more strict constraints are dictated by the physics of the problem. As we argue in the main text, for $r_0 = 0$ the large-$\mathbf{Q}$ asymptote of the function F should be $F(\mathbf{Q}) \propto Q^{-3N/2+1-s}$. Then, for $N = 4$ the walker distribution function scales at large $\mathbf{Q}$ as $f(\mathbf{Q}) = F(\mathbf{Q})/g(\mathbf{Q}) \propto Q^{-4-s-\alpha-3\beta}$ and convergence of $\int f(Q)Q^8 dQ$ requires $\alpha+3\beta+s > 5$. The same type of convergence condition should also hold for the four- and three-body subsystems of the 4+1 problem. These three conditions can be written simultaneously as

$$\alpha + (N-1)\beta > -s_{N+1} + 3N/2 - 1, \tag{S12}$$

where s_{N+1} denotes the parameter s for the $N+1$ body (sub)system with $N = 2$, 3, and 4 [see Fig.2(b) of the main text]. We should also mention that the condition (S12) holds for the pure tetramer and trimer calculations, assuming, respectively, $g(\mathbf{q}_1,\mathbf{q}_2) \propto (q_1^2+q_2^2)^{\frac{\alpha}{2}} q_1^\beta q_2^\beta/\kappa$ and $g(\mathbf{q}_1) \propto q_1^{\alpha+\beta}/\kappa$.

Trying various combinations of α and β we have checked that the result for the energy does not depend on these parameters as long as they satisfy (S12) and as long as we use sufficiently large N_w. However, for some combinations of α and β the calculation of the exponent s should be done with care. This problem arises due to the fact that we are dealing with finite E and a. Then the large-Q asymptote of $F(\mathbf{Q})$ at fixed hyperangle $\hat{\mathbf{Q}}$ and the large-Q asymptote of the integral $\int F(\mathbf{Q})d\hat{\mathbf{Q}}$ do not necessarily coincide. To make this point more clear consider the two-dimensional function $1/[(1+x^2)(1+y^2)]$. For any fixed hyperangle $\theta = \arctan(x/y)$ larger than 0 and smaller than $\pi/2$ this function asymptotes to $\propto 1/\rho^4$ at large hyperradius $\rho = \sqrt{x^2+y^2}$. However, if $\theta = 0$ or $\pi/2$, we obtain the $1/\rho^2$ scaling. Moreover, if we integrate $1/[(1+x^2)(1+y^2)]$ over θ, we obtain yet another power law $\propto 1/\rho^3$.

Clearly, the power-law scaling that one obtains from a function of the type $(x^2+y^2)^{\frac{\alpha}{2}} x^\beta y^\beta/[(1+x^2)(1+y^2)]$ depends on α, β, and on the exact limiting procedure. A possible solution of this problem is to restrict α and β such that the total integral over the hyperangles is properly behaved. In the particular example just considered we have to choose β such that the integral $x^\beta/(1+x^2)$ diverges at large x, i.e., $\beta > 1$, thus effectively depreciating the role of the small-x region. A much simpler solution is to restrict the hyperangular integration to the region $\epsilon < \theta < \pi/2 - \epsilon$. This is what we do in the actual calculations. Namely, when we gather statistics on walkers in the interval $(Q, Q+\delta Q)$, we update the bin value only if $q_i/Q > \epsilon$.