D-dimensional three-body bound-state problem with zero-range interactions

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(Received 24 November 2021; revised 6 July 2022; accepted 2 August 2022; published 16 August 2022)

We solved analytically the three-body mass-imbalanced problem embedded in D dimensions for zero-range resonantly interacting particles. We derived the negative energy eigenstates of the three-body Schrödinger equation by imposing the Bethe-Peierls boundary conditions in D dimensions for zero-energy two-body bound states. The solution retrieves the Efimov-like discrete scaling factor dependence with dimension. The analytical form of the mass-imbalanced three-body bound-state wave function can be used to probe the effective dimension of asymmetric cold atomic traps for Feshbach resonances tuned close to the Efimov limit.

DOI: 10.1103/PhysRevA.106.023311

I. INTRODUCTION

Magnetically tunable Feshbach resonances in ultracold atomic gases open up several possibilities to explore few- and many-body physics [1]. Access to the universal regime, therein the scattering length exceeding in magnitude all other length scales of the system, was a significant breakthrough in cold atom physics [2–4]. Not only can the interactions and energies be freely tuned in ultracold atomic traps, but also the geometry of the system. The ability of squeezing the shape of the atomic cloud opens new opportunities for studies of few-body effects in such engineered systems.

In the context of few-body problems, one intriguing phenomenon is the Efimov effect [5–7]. It consists of an infinite series of weakly bound three-body states following a universal geometrical scaling law close to the two- or three-body threshold. Several ultracold atomic experiments have by now observed the Efimov effect in homo- [8–11] and heteronuclear systems [12–14]. In dilute gases, weakly bound Efimov trimer states mediate inelastic collisions giving rise to a rich spectrum of atom loss resonances as a function of the tunable scattering length. The universal aspects of Efimov physics, first proposed in the nuclear physics context, appear over an incredible variety of systems covering a wide range of physical scales: atomic gases [15], Bose polarons [16,17], dipolar molecules [18], and strongly interacting photons [19], to name a few examples.

Despite many advances in theory and experiments, which allow the continuous changing of the geometry of the system and the effective dimension of the trap, associating the Efimov geometrical scaling with a squeezed system remains an important property yet to be observed. Historically, the determinant role of the dimension to establish the Efimov effect is known theoretically—as predicted in the early 1980s [20,21], the Efimov effect exists in three dimensions but is absent in two. The possibility to experimentally observe this prediction only appeared after the construction of Bose-Einstein condensates in traps with one [22] and two [23] dimensions. This experimental advancement brought together technologies which allowed a continuous modification the geometry of the cloud.

The independent and continuous change of one spatial dimension of the trap, allied to the careful control of the scattering length, could potentially lead to the observation of a change in the Efimov geometrical ratio associated with an *effective dimension*. The separation of successive peaks in the three-body recombination loss [11], or even by measuring directly the binding energies of the trimers [24], are one of the possible observables to probe and study the vicinity of the vanishing of the Efimov effect. However, in a trapped system the successive ratios between trimer states may not be necessarily the same, but could depend nontrivially on the properties of Feshbach resonances [25]. Therefore, one should be cautious when associating the separation between recombination peaks or Efimov states to the noninteger dimension in squeezed traps.

Despite lacking clear experimental evidence, studies of three-body systems in reduced geometries have been the subject of interest in recent years. Different approaches were employed to study the dimensional effects in three-body systems close to the Efimov limit. This limit is achieved when the dimer binding energy vanishes or, equivalently, the scattering length is driven to infinity, which is also known as a unitary limit. In such studies, the system is embedded in a fractional dimension D [2,26–30], in mixed dimensions [31–33], in which atoms move in different spatial dimensions, or it is squeezed to lower dimensions by changing the shape of an external potential [34–38]. An approximate relation between the noninteger dimension D used in this paper to the squeezing in one direction by an external potential was already derived in Ref. [39], $b_{\rm ho}^2/r_{\rm 2D}^2 = 3(D-2)/(3-D)(D-1)$, where $b_{\rm ho}$ is the harmonic oscillator parameter and is represented in units of the rms radius of the three-body system in two dimensions $r_{\rm 2D}$.

In this paper, we provide an analytical solution for the bound-state wave function with finite binding energy for the resonant three-body mass-imbalanced problem in D dimensions. The calculation uses the Bethe-Peierls (BP) boundary condition approach [40], for each pair of resonant particles in the three-body system, extended to arbitrary dimensions. For $D = 3$, this was the method originally used by Efimov to solve the three-boson problem leading to the discovery of the geometrical ratio of the binding energies [5,7].

The method adopted here follows closely Efimov's solution in coordinate space using hyperspherical coordinates, which is now applied to three distinct particles in D dimensions. In this case of a zero-range interaction, each Faddeev component of the wave function is an eigenstate of the free Schrödinger eigenvalue equation for a given binding energy. The BP boundary conditions are imposed on the full wave function, obtained by summing the three Faddeev components, to account for the zero-range interaction.

The Efimov scaling parameter is obtained from the solution of a transcendental equation in D dimensions, which comes from the Faddeev components of the wave function for three different particles. The Efimov parameter appears naturally in each Faddeev component as a direct consequence of a system of homogeneous linear equations. For the particular case of two identical bosonic particles and a distinct one, we reproduce the previous results of Ref. [27] obtained with the momentum space representation.

The analytical solution of the eigenvalue equation for the three-body bound-state wave function opens the possibility for future explorations of different observables, such as the three-body radius [41] and the momentum densities [42,43], uncovering analytically the scaling laws of these quantities with the binding energy and dimension. Such scaling laws, in correspondence with limit cycles, evidence the crucial importance of the effective dimension on the Efimov physics and point to the direction for experimental investigations.

II. BETHE-PEIERLS BOUNDARY CONDITION IN *D* DIMENSIONS

We derive the BP boundary condition considering a system of two nonrelativistic spinless particles in D dimensions with a short-range s-wave interaction. For relative distances beyond a finite range, two particles are noninteracting and the radial wave function of the pair, working in units of $\hbar = 1$, is known to be [44]

$$R(r) = \sqrt{\frac{\pi}{2p}}\, r^{1-\frac{D}{2}}\left[\cot\delta_D(p) J_{\frac{D}{2}-1}(pr) - Y_{\frac{D}{2}-1}(pr)\right], \tag{1}$$

where p is the relative momentum, $J_{D/2-1}$ and $Y_{D/2-1}$ are the Bessel functions of the first and second kind, and the s-wave phase shift $\delta_D(p)$ is given in terms of the scattering length a as

$$\cot\delta_D(p) = \frac{Y_{\frac{D}{2}-1}(pa)}{J_{\frac{D}{2}-1}(pa)}. \tag{2}$$

The Bethe-Peierls boundary condition at zero energy for the contact interaction can now be obtained by taking the limit to the origin of the logarithmic derivative of the reduced wave function $u(r) = r^{(D-1)/2} R(r)$,

$$\left[\frac{d}{dr}\ln u(r)\right]_{r\to 0} = \left[\frac{D-1}{2r} - \frac{D-2}{r - r(r/a)^{D-2}}\right]_{r\to 0}, \tag{3}$$

which reproduces the well-known results

$$\left[\frac{d}{dr}\ln u(r)\right]_{r\to 0} = \begin{cases} -\frac{1}{a}, & \text{for } D = 3,\\ \frac{1}{2r} - \frac{1}{\ln(r/a)}, & \text{for } D = 2. \end{cases} \tag{4}$$

We use Eq. (3) to obtain the solution of the three-body Schrödinger equation in the unitary limit.

III. THREE-BODY MASS-IMBALANCED PROBLEM

We consider three different bosons with masses m_i, m_j, m_k, and coordinates $\mathbf{x}_i$, $\mathbf{x}_j$, and $\mathbf{x}_k$. One can eliminate the center-of-mass coordinate and describe the system in terms of two relative Jacobi coordinates. One can identify three sets of such coordinates,

$$\boldsymbol{r}_i = \mathbf{x}_j - \mathbf{x}_k \quad \text{and} \quad \boldsymbol{\rho}_i = \mathbf{x}_i - \frac{m_j\mathbf{x}_j + m_k\mathbf{x}_k}{m_j + m_k}, \tag{5}$$

where (i, j, k) are taken cyclically among (1,2,3). One can choose any of such sets of coordinates to solve the three-body Schrödinger equation. The Faddeev decomposition of the three-body wave function $\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)$ amounts to writing it as a sum of three two-body wave functions, $\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \psi^{(1)}(\boldsymbol{r}_1, \boldsymbol{\rho}_1) + \psi^{(2)}(\boldsymbol{r}_2, \boldsymbol{\rho}_2) + \psi^{(3)}(\boldsymbol{r}_3, \boldsymbol{\rho}_3)$, where we omitted the center-of-mass plane wave. Each component satisfies the free Schrödinger eigenvalue equation.

$$\left[\frac{1}{2\eta_i}\nabla^2_{\boldsymbol{r}_i} + \frac{1}{2\mu_i}\nabla^2_{\boldsymbol{\rho}_i} - E\right]\psi^{(i)}(\boldsymbol{r}_i, \boldsymbol{\rho}_i) = 0, \tag{6}$$

where E is the system energy and the reduced masses are given by $\eta_i = m_j m_k/(m_j + m_k)$ and $\mu_i = m_i(m_j + m_k)/(m_i + m_j + m_k)$. The BP boundary condition applies to the total wave function; when applied to the chosen coordinates pair $(\boldsymbol{r}_i, \boldsymbol{\rho}_i)$, it reads, in the unitary limit $a \to \infty$,

$$\left[\frac{\partial}{\partial r_i} r_i^{\frac{D-1}{2}} \Psi(\boldsymbol{r}_i, \boldsymbol{\rho}_i)\right]_{r_i\to 0} = \frac{3-D}{2}\left[\frac{\Psi(\boldsymbol{r}_i, \boldsymbol{\rho}_i)}{r_i^{\frac{3-D}{2}}}\right]_{r_i\to 0}. \tag{7}$$

This solution strategy was applied to different particles and spins in Ref. [45] and we adapt it to D dimensions following closely Efimov's original derivation [5,7].

For convenience, we can simplify the form of the kinetic energies by introducing the new coordinates

$$\boldsymbol{r}'_i = \sqrt{\eta_i}\,\boldsymbol{r}_i \quad \text{and} \quad \boldsymbol{\rho}'_i = \sqrt{\mu_i}\,\boldsymbol{\rho}_i. \tag{8}$$

The three sets of primed coordinates are related to each other by the orthogonal transformations

$$\boldsymbol{r}'_j = -\boldsymbol{r}'_k\cos\theta_i + \boldsymbol{\rho}'_k\sin\theta_i, \quad \boldsymbol{\rho}'_j = -\boldsymbol{r}'_k\sin\theta_i - \boldsymbol{\rho}'_k\cos\theta_i, \tag{9}$$

where $\tan\theta_i = [m_i M/(m_j\, m_k)]^{1/2}$, with $M = m_1 + m_2 + m_3$. For bosons in the partial-wave channel with vanishing total angular momentum, one can define the reduced Faddeev component as

$$\chi_0^{(i)}(r'_i, \rho'_i) = (r'_i\,\rho'_i)^{\frac{D-1}{2}}\,\psi^{(i)}(r'_i, \rho'_i). \tag{10}$$

The corresponding Schrödinger equation for $\chi_0^{(i)}$ is separable in the hyperspherical coordinates $r_i' = R\sin\alpha_i$ and $\rho_i' = R\cos\alpha_i$, so that one can write

$$\chi_0^{(i)}(R,\alpha_i) = C^{(i)}F(R)G^{(i)}(\alpha_i), \tag{11}$$

where $R^2 = r_i'^2 + \rho_i'^2$ and $\alpha_i = \arctan(r_i'/\rho_i')$, with $F(R)$ and $G^{(i)}(\alpha_i)$ satisfying the following equations,

$$\left[-\frac{\partial^2}{\partial R^2} + \frac{s_n^2 - 1/4}{R^2} + \kappa_0^2\right]\sqrt{R}F(R) = 0, \tag{12}$$

$$\left[-\frac{\partial^2}{\partial \alpha_i^2} - s_n^2 + \frac{(D-1)(D-3)}{\sin^2 2\alpha_i}\right]G^{(i)}(\alpha_i) = 0, \tag{13}$$

where $-\kappa_0^2 = 2E$, and s_n is the Efimov parameter, to be determined by the BP boundary condition.

The definitions $z = \cos 2\alpha_i$ and $G^{(i)} = (1-z^2)^{1/4}g^{(i)}$ turn Eq. (13) into the form of the associated Legendre differential equation [46] with the known analytical solutions

$$G^{(i)}(\alpha_i) = \sqrt{\sin 2\alpha_i}\Big[P^{D/2-1}_{s_n/2-1/2}(\cos 2\alpha_i) - \frac{2}{\pi}\tan[\pi(s_n-1)/2]Q^{D/2-1}_{s_n/2-1/2}(\cos 2\alpha_i)\Big], \tag{14}$$

where $P_n^m(x)$ and $Q_n^m(x)$ are the associated Legendre functions. We have imposed the boundary condition that guarantees a finite value for the Faddeev component $\psi^{(i)}$ at $\rho_i = 0$, which leads the reduced wave function to satisfy $\chi_0^{(i)}(r_i', \rho_i' = 0) = 0$. In terms of the hyperspherical coordinates, it leads to $G^{(i)}(\alpha_i = \pi/2) = 0$, since $\rho_i' = R\cos\alpha_i$.

Therefore, the solution for $\psi^{(i)}(r_i', \rho_i')$ is given by

$$\psi^{(i)}(r_i',\rho_i') = C^{(i)}\frac{K_{s_n}\left(\kappa_0\sqrt{r_i'^2+\rho_i'^2}\right)}{\left(r_i'^2+\rho_i'^2\right)^{D/2-1/2}}\frac{\sqrt{\sin[2\arctan(r_i'/\rho_i')]}}{\{\cos[\arctan(r_i'/\rho_i')]\sin[\arctan(r_i'/\rho_i')]\}^{D/2-1/2}} \times\left[P^{D/2-1}_{s_n/2-1/2}\{\cos[2\arctan(r_i'/\rho_i')]\} - \frac{2}{\pi}\tan[\pi(s_n-1)/2]Q^{D/2-1}_{s_n/2-1/2}\{\cos[2\arctan(r_i'/\rho_i')]\}\right], \tag{15}$$

where K_{s_n} is the modified Bessel function of the second kind.

One obtains the Efimov parameter s_n by considering that all three pairs of particles are resonant. Then, the BP boundary condition, Eq. (7), should be satisfied by the three-body wave function when each relative distance between two of the particles tends to zero, namely $r_i = R\sin\alpha_i \to 0$, implying that $\alpha_i \to 0$ for finite hyper-radius R. The hyper-radial part of the wave function factorizes in the BP boundary condition for each r_i, which depends only on the hyperangular part of each Faddeev component (14). The resulting homogeneous linear system for the coefficients $C^{(i)}$ reads

$$\frac{C^{(i)}}{2}\left[(\cot\alpha_i)^{\frac{D-1}{2}}\left(\sin 2\alpha_i\frac{\partial}{\partial\alpha_i} + D - 3\right)G^{(i)}(\alpha_i)\right]_{\alpha_i\to 0} + (D-2)\left[\frac{C^{(j)}G^{(j)}(\theta_k)}{(\sin\theta_k\cos\theta_k)^{\frac{D-1}{2}}} + \frac{C^{(k)}G^{(k)}(\theta_j)}{(\sin\theta_j\cos\theta_j)^{\frac{D-1}{2}}}\right] = 0, \tag{16}$$

for $i \neq j \neq k$. Taking the three cyclic permutations of $\{i, j, k\}$, one has a homogeneous system of three linear equations, from which one obtains the Efimov parameter s_n by solving the characteristic transcendental equation.

We remark that the key point of this paper is the analytical solution, for finite energies, of each Faddeev component for bound-state systems of the three distinct particles—this situation is more complex than our previous work given in Ref. [27]. The use of the BP boundary condition results in Eq. (15) and, in order to fully define the wave function, Eq. (16) should be solved to determine the Efimov parameter s_n and the relative weights $C^{(i)}$ of the Faddeev components of the wave function.

In the case of a purely imaginary value for the s_n parameter, the effective potential in Eq. (12) is attractive, giving rise to the well-known pathological $1/R^2$ interaction. This potential admits a solution at any energy with a spectrum "unbounded from below," a phenomenon discovered long ago by Thomas [47] and referred to as the "Thomas collapse." In particular, the transcendental equation in three dimensions reduces to Efimov's one for identical bosons [6], and in the general case of different particles to the one derived by Bulgac and Efimov [7,45], when the spin is neglected. In these cases the wave function (15) presents the characteristic log periodicity.

The most favorable conditions for the existence of Efimov-like log-periodic solutions occur for spinless particles with a zero-energy two-body bound state with zero angular momentum. The particular case where only two pairs interact resonantly is easily implemented, being necessary only to drop one of the equations in Eq. (16) and set to zero the Faddeev component corresponding to the nonresonant pair. This method may be used also for particles with spin.

IV. RESULTS AND DISCUSSIONS

The present method applies to the bound state of three distinct particles for dimensions $D > 2$, where the homogeneous linear system in Eq. (16) admits nontrivial solutions with purely imaginary values $s_n \to is_0$, i.e., in the Efimov region. That happens only for a given range of dimensions $2 < D < 4$ constrained by the condition that $s_0(D) \to 0$, which also depends on the mass imbalance in the system. Here, we discuss some alternative examples of triatomic systems composed by ^{6}Li, ^{23}Na, ^{87}Rb, and ^{133}Cs in D dimensions from the solution of Eq. (16), which besides s_n provides the relative weights $C^{(i)}$

TABLE I. Range of D, $D_c^< < D < D_c^>$, and critical values of the trap parameter allowing Efimov states for some examples of mass-imbalanced systems.

System	$b_{ho}^</r_{2D}$	$D_c^<$	$D_c^>$
^{6}Li$_3$	0.988	2.297	3.755
^{6}Li-^{23}Na$_2$	0.959	2.282	3.814
^{6}Li-^{23}Na-^{133}Cs	0.896	2.251	3.852
^{6}Li-^{87}Rb$_2$	0.882	2.244	3.929
^{6}Li-^{87}Rb-^{133}Cs	0.864	2.235	3.938
^{6}Li-^{133}Cs$_2$	0.856	2.231	3.954

of the Faddeev components, Eq. (15), and allows us to obtain the configuration space wave function that will be explored in one example in what follows.

In Table I for some choices of mass-imbalanced systems, we show the range of D values, $D_c^< < D < D_c^>$, and the critical value of the trap parameter for which the Efimov effect is present. The results in the table reveal that as the mass imbalance increases to heavy-heavy-light, the range of D values for the existence of the Efimov effect widens. For two infinitely heavy masses, the lowest critical dimension tends to $D = 2$ from above, i.e., $D_c^< \to 2_+$, while the trap parameter tends to zero. The maximum critical dimension in that case tends to $D = 4$ from below, i.e., $D_c^> \to 4_-$, and the trap length parameter to infinity. Such subtle behavior is clearly seen in Table I following the pattern from ^{6}Li-^{23}Na$_2$ to ^{6}Li-^{133}Cs$_2$ passing through a fully mass-imbalanced system. When one of the ^{133}Cs is substituted by a lighter atom, as in ^{6}Li-^{23}Na-^{133}Cs, the region for Efimov states shrinks. We observe that among the examples we have discussed, the smallest range of dimensions for the existence of the Efimov effect is found for three identical atoms. In this case the squeezing length in units of the rms radius in two dimensions is given by $b_{ho}/r_{2D} = 0.988$, and in this trap configuration the Efimov effect vanishes for three identical atoms.

Figure 1 displays the geometrical ratio between two successive Efimov states as a function of D for the systems given in Table I. Noteworthy in the figure, the ratio of the energies

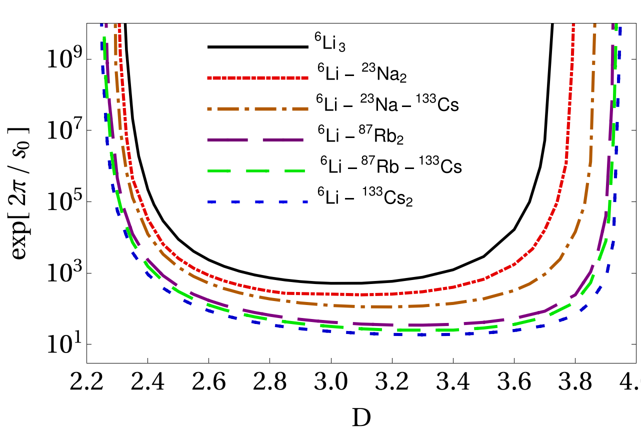

FIG. 1. Efimov scale parameter as a function of the effective dimension for several mass-imbalanced system's configuration.

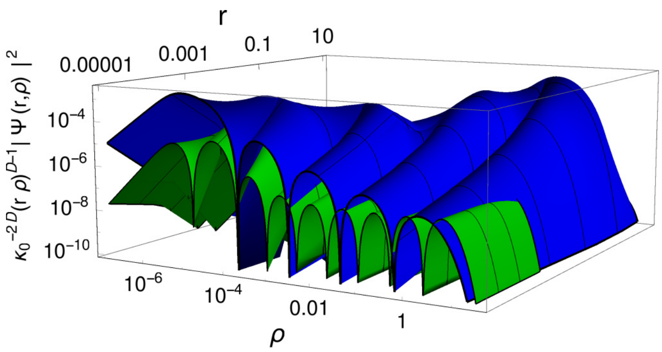

FIG. 2. Dimensionless radial distribution as a function of dimensionless quantities $r = \kappa_0 r_3$ (^{133}Cs-^{87}Rb relative distance) and $\rho = \kappa_0 \rho_3$ (^{6}Li relative distance to the ^{133}Cs-^{87}Rb system). We consider the three-body system ^{6}Li-^{133}Cs-^{87}Rb for $D = 2.5$ (blue) with $b_{ho}/r_{2D} = \sqrt{2}$, and $D = 3.0$ (green). The angle between $\vec{r}$ and $\vec{\rho}$ is fixed to $\pi/3$.

of two successive Efimov states varies up to $+\infty$, while large mass asymmetries favor ratios smaller than those for $D = 3$.

Figure 2 displays the radial distribution of the ^{6}Li-^{133}Cs-^{87}Rb molecule for $D = 2.5$ and $D = 3.0$, represented respectively by the blue and green surfaces. The physical realization of $D = 2.5$ corresponds to a squeezed trap with $b_{ho}/r_{2D} = \sqrt{2}$, having a ratio between energies of successive shallowest states at unitarity given by 202 ($s_0 = 1.183\,29$). We recall that for $D = 3$, $s_0 = 2.005\,88$ and 22.9 for the energy ratio. It is possible to observe log-periodic behavior, a fingerprint of an Efimov-like state. The nodes of the wave function in the ρ coordinate are located at $\rho_{n+1} \sim e^{\pi/s_0}\rho_n$, and, as expected, the location depends on D [27]. The oscillations in the r direction, although not visible in the figure, are present due to the log periodicity of the Faddeev component of the wave function coming from $K_{\imath s_0}(\kappa_0\sqrt{r_i'^2 + \rho_i'^2})$ when $\kappa_0\sqrt{r_i'^2 + \rho_i'^2}$ attains small enough values.

V. SUMMARY

We presented an analytical solution of the mass-imbalanced three-body problem in D dimensions in the Efimov limit. Use of the Bethe-Peierls boundary condition allowed us to formulate this problem and in particular show how to compute the Efimov parameter for a wide range of mass ratios and dimensions. The importance in having a relatively simple, analytical way to compute the wave function for a finite three-body energy opens up the possibility to probe the Efimov physics in ultracold atomic systems through radio-frequency spectroscopy [42]. Such a technique has been used in Ref. [48] to measure Tan's contact parameters [49], which can be associated with the thermodynamic properties of the system. Quite recently, the two-body contact was measured across the superfluid transition of a planar Bose gas [50].

Within the perspective of our work, two- and three-body contacts can be computed for mass-imbalanced systems in D dimensions using Eq. (12) by generalizing other known techniques [43], which were applied to three identical bosons in three dimensions. The contacts will also allow us to address the intriguing phenomenon present in the crossover of the discrete and continuum scale symmetry by decreasing the effective dimension. Then, the system evolves from $D = 3$ to $D = 2$, for which the Efimov effect disappears—in this transition, the log-periodicity of the wave function gives place to a power-law behavior. Such an exciting possibility suggests that the realization of an atomic analogy to "unnuclear" systems [51], namely "unatomic" states, may occur in cold traps squeezed from three to two dimensions. We leave the study of such a possibility for future work.

ACKNOWLEDGMENTS

This work was partially supported by Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP) [Grants No. 2019/00153-8 (M.T.Y.), No. 2017/05660-0 (T.F.), No. 2020/00560-0 (D.S.R.), and No. 2018/25225-9 (G.K.)], and Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) [Grants No. 308486/2015-3 (T.F.), No. 303579/2019-6 (M.T.Y.), and No. 309262/2019-4 (G.K.)].

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