Efimov effect in quantum magnets

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Physics is said to be universal when it emerges regardless of the underlying microscopic details. A prominent example is the Efimov effect, which predicts the emergence of an infinite tower of three-body bound states obeying discrete scale invariance when the particles interact resonantly. Because of its universality and peculiarity, the Efimov effect has been the subject of extensive research in chemical, atomic, nuclear and particle physics for decades. Here we employ an anisotropic Heisenberg model to show that collective excitations in quantum magnets (magnons) also exhibit the Efimov effect. We locate anisotropy-induced two-magnon resonances, compute binding energies of three magnons and find that they fit into the universal scaling law. We propose several approaches to experimentally realize the Efimov effect in quantum magnets, where the emergent Efimov states of magnons can be observed with commonly used spectroscopic measurements. Our study thus opens up new avenues for universal few-body physics in condensed matter systems.

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Here \( \nabla^i_\epsilon \) is an operator to displace \( \mathbf{r}_i \) to \( \mathbf{r}_i + \epsilon \) and a constant energy shift \( - (6S J_1 - 6S J_2 - 2SD + D + B) N \) is omitted in the right hand side.

The emergence of the Efimov effect in quantum magnets can be understood intuitively by using an exact mapping between spins and bosons, which is known as the Holstein–Primakoff transformation\(^{25}\). It is clear from the Schrödinger equation that \( J \) in the first term acts as a hopping amplitude and gives a single-magnon dispersion relation:

\[
E_0(\mathbf{k}) = \sum_i S J [1 - \cos(\mathbf{k} \cdot \mathbf{\hat{e}})]
\]  

The rest describe interactions between a pair of magnons where \( J_i > J \) and \( D > 0 \) act as nearest-neighbour and on-site attractions, respectively. (Note that the effective \( N \)-magnon hardcore repulsion also exists for \( N = 2S + 1 \) according to \( (S^2)_{2S+1} = 0 \). By setting \( \mathbf{r}_1 = \cdots = \mathbf{r}_N \) in equation (3), we obtain \( E = 3N(N - 1)J + N(N - 1)D \Psi(\mathbf{r}, \ldots, \mathbf{r}) = 0 \). Therefore, unless \( E = 3N(N - 1)J + N(N - 1)D = 0 \), the constraint \( \Psi(\mathbf{r}, \ldots, \mathbf{r}) = 0 \) is automatically satisfied. In particular, \( D \) plays no role for \( S = 1/2 \) as \( \Psi(\mathbf{r}, \mathbf{r}) = 0 \). By tuning these couplings, we can induce a scattering resonance between two magnons. Once the two-magnon resonance is achieved, three magnons should exhibit the Efimov effect (1) because the Efimov effect is universal in the sense that it emerges regardless of microscopic details.

Two-magnon resonance

We start with a scattering problem of two magnons. A two-magnon solution with a centre-of-mass momentum \( \mathbf{K} \) is written as

\[
\Psi(\mathbf{r}_1, \mathbf{r}_2) = e^{i \mathbf{K} \cdot \mathbf{R}} \psi_\mathbf{K}(\mathbf{\rho})
\]

where \( \mathbf{R} \equiv (\mathbf{r}_1 + \mathbf{r}_2)/2 \) and \( \mathbf{\rho} \equiv \mathbf{r}_1 - \mathbf{r}_2 \) are centre-of-mass and relative coordinates, respectively. The Bose statistics of magnons implies \( \psi_\mathbf{K}(\mathbf{\rho}) = \psi_\mathbf{K}(-\mathbf{\rho}) \) for the relative wave function. The two-magnon Schrödinger equation can be solved in a standard way by bringing it into the Lippmann–Schwinger equation (see Methods for details).

The scattering resonance between two magnons is defined by the divergence of the s-wave scattering length \( a_s \) where a two-magnon bound state appears from the continuum. \( a_s \) can be inferred from the asymptotic behaviour of the wave function at zero energy and zero centre-of-mass momentum:

\[
\lim_{|\mathbf{\rho}| \to \infty} \Psi_0(\mathbf{\rho})|_{E=0} \propto 1 - \frac{a_s}{|\mathbf{\rho}|}
\]

By matching this asymptotic behaviour with the obtained solution (equation (7) in Methods), the analytic expression of \( a_s \) is obtained as

\[
a_s = \frac{2S - 1 + \frac{3}{2} \left( 1 - \frac{D}{J} - \frac{J}{D} \right) \frac{1}{3} \left( 1 - \frac{D}{J} - \frac{J}{D} \right)}{2S - 1 + \frac{3}{2} \left( 1 - \frac{D}{J} - \frac{J}{D} \right) \frac{1}{3} \left( 1 - \frac{D}{J} - \frac{J}{D} \right)}
\]

Here \( a \) is the lattice constant and \( W \equiv (\sqrt{6}/96\pi^4) \Gamma(1/24) \Gamma(5/24) \Gamma(7/24) \Gamma(11/24) = 0.505462 \) results from one of the Watson’s triple integrals\(^{26}\).

As a consequence, we find that the two-magnon resonance \( a_s \rightarrow \infty \) takes place at \( J_s/J = 2.93654 \) for \( S = 1/2 \). Critical anisotropies for other spins are shown in Fig. 1. In particular, the two-magnon resonance for \( S = 1 \) is induced by the exchange anisotropy at \( J_s/J = 4.87307 \) (\( D = 0 \)), whereas it is induced by the single-ion anisotropy at \( D/J = 4.76874 \) (\( J_s = f \)) or \( D/J = 5.12703 \) (\( J_s = -f \)) for an isotropic ferromagnetic or antiferromagnetic coupling, respectively. Above these critical points, two magnons form an s-wave bound state at \( \mathbf{K} = 0 \). Its binding energy \( E < 0 \) determines the three-magnon threshold in Figs 2 and 3.
Three-magnon Efimov effect

We now turn to a bound-state problem of three magnons. A bound-state solution to the three-magnon Schrödinger equation can be obtained in a similar way to the previous two-magnon problem (see Methods for details). Because our purpose here is to demonstrate the Efimov effect of magnons, we focus on the s-wave channel at zero centre-of-mass momentum where the Efimov effect is supposed to emerge.

We find that three magnons form a series of bound states and their binding energies are shown in Table 1 right at the anisotropy-induced two-magnon resonances located above. The ratios of two successive binding energies obey the universal scaling law (1), which supports that the observed bound states of three magnons are indeed the Efimov states. Note that although the Efimov effect emerges only in the s-wave channel, it is in general possible that there are non-Efimov three-magnon bound states in other channels, which may have lower binding energies.

In the case of $S = 1/2$, the two lowest binding energies near the two-magnon resonance are shown in Fig. 2. The universal theory predicts that the spectrum of Efimov states is completely characterized by the s-wave scattering length $a_s$ and the so-called Efimov parameter $\kappa_s$ (ref. 4):

$$E_n \to -\lambda^{-2n} \frac{\hbar^2 \kappa_s^2}{m} F\left(\frac{\lambda^n}{\kappa_s a_s}\right) \quad (n \to \infty)$$

Here $m$ is the mass of constituent particles and $F(x)$ is the universal function defined in a range $-0.663293 \leq x \leq 14.1314$ and normalized as $F(0) = 1$. The inverse effective mass of magnons is $1/m = 25\lambda^2/\hbar^2$, which is inferred from the single-magnon dispersion relation (4). By matching equation (6) with the binding energy of the second excited state at the resonance, we obtain

$$\kappa_s a_s \simeq 0.463.$$  The resulting universal curves for $n = 0$ and $n = 1$ are also plotted in Fig. 2 by using $a_s$ obtained in equation (5). We find an excellent agreement of the binding energy of the first excited state with the universal theory, which leaves no doubt that this three-magnon bound state is the universal Efimov state. On the other hand, the binding energy of the ground state deviates from the universal theory away from the two-magnon resonance where non-universal corrections become non-negligible.

Similarly, in the case of $S = 1$ with $J_z = J (-J)$, we obtain $\kappa_s a_s \simeq 0.173$ (0.0478) by matching equation (6) with the binding energy of the first excited state at the resonance. The resulting universal curve for $n = 0$ is plotted in Fig. 3 as well as the ground-state binding energy near the two-magnon resonance. We find a reasonable agreement between them, which confirms that this three-magnon bound state is consistent with the universal Efimov state. Our findings here support the fact that resonantly interacting magnons fall into the class of universal few-body systems. Accordingly, other universal aspects of Efimov physics, such as a pair of four-body resonances associated with every Efimov state$^{27,28}$, also apply to the system of magnons.

Towards experimental realization

In summary, we showed that magnons in quantum magnets exhibit the Efimov effect by tuning an easy-axis exchange or single-ion anisotropy. The single-ion anisotropy $D$ can be changed significantly in organic magnets by choosing different ligands$^{29}$. Therefore, it is possible to find a compound with spin $S \geq 1$ whose $D/J$ ratio is already close to the critical value. For example, there is an $S = 1$ ferromagnetic compound based on molecular Ni$_2$S$_2$ squares with $D/J \simeq 3.0(5)$ (ref. 30), which is not far from the critical value 4.76874. Furthermore, the exchange coupling $J$ can be tuned with pressure$^{31}$ to bring the system near the two-magnon resonance and realize the Efimov effect.

On the other hand, the single-ion anisotropy plays no role for $S = 1/2$. In this case, the two-magnon resonance can be induced by the exchange anisotropy, although it is in general difficult to tune and its critical value ($J_z/J = 2.93654$) is somewhat large. However, the critical exchange anisotropy can be reduced significantly if the magnet is spatially anisotropic. Spatially anisotropic exchange couplings can be taken into account simply by replacing $J_z$ and $J_{\perp}$ in the Hamiltonian (2) with $J_z$ and $J_{\perp}$ respectively. We assume a uniaxial anisotropy $J_z = J' = J$ and $J_{\perp} = J''$ with a shared ratio $\gamma = J'/J'' = J_z/J_{\perp}$. As shown in Fig. 4, the corresponding critical exchange anisotropy reduces significantly towards an isotropic point $J_z/J \to 1$ in a quasi-one-dimensional ($\gamma \to 0$) or two-dimensional ($\gamma \to \infty$) limit. Because magnets with strong spatial anisotropies are very common$^{2-38}$, there is hope to find an $S = 1/2$ ferromagnetic compound whose $J_z/J$ ratio is already close to the

| $S$ | $J_z/J$ | $D/J$ | $n$ | $E_n/J$ | $\sqrt{E_{n-1}/E_n}$ |
|-----|--------|------|----|--------|-------------------|
| 1/2 | 2.93654 | —    | 0  | $-2.09 \times 10^{-1}$ | —                 |
|     |        | 1    | $-4.15 \times 10^{-4}$ | 22.4               |
|     | 4.87307 | 0    | 2  | $-8.08 \times 10^{-7}$ | 22.7               |
| 1   | 4.76874 | 0    | 1  | $-5.61 \times 10^{-1}$ | —                 |
| 1   | +1     | 0    | 2  | $-1.02 \times 10^{-3}$ | 22.4               |
| 1   | —1     | 0    | 2  | $-2.00 \times 10^{-6}$ | 22.7               |
| 1   | 5.12703 | 0    | 1  | $-3.61 \times 10^{-3}$ | —                 |
| 1   | —1     | 0    | 2  | $-8.88 \times 10^{-6}$ | 22.2               |
critical value. Once such a compound is identified, the spatial anisotropy $\gamma$ can be tuned with pressure. An alternative approach to induce the two-magnon resonance in $S = 1/2$ magnets even without the exchange anisotropy ($J_z = J$) is to introduce frustrated exchange interactions. The simplest example is given by quasi-one-dimensional spin chains with nearest-neighbour ferromagnetic and next-nearest-neighbour antiferromagnetic couplings:

$$H_{\text{inter}} = -\sum_i (J_i^z S_i \cdot S_{i+4} - J_i^{2z} S_i \cdot S_{i+2z})$$

which are realized in Rb$_2$CuMo$_3$O$_{12}$ (ref. 39), LiCuVO$_4$ (ref. 40) and Li$_2$CuO$_2$ (ref. 41). When $J_i^z/J_i^{2z} < 4$, the single-magnon dispersion develops minima at nonzero momentum $K_0 = \pm \arccos(J_i^z/J_i^{2z})$, and accordingly, two magnons form a bound state with a centre-of-mass momentum $2K_0$ (refs 41–47). This two-magnon bound state disappears into the continuum at a certain interchain coupling:

$$H_{\text{inter}} = -\sum_{\sigma} (S_{\sigma} \cdot S_{\sigma+4} + S_{\sigma} \cdot S_{\sigma+9})$$

which leads to the two-magnon resonance. The corresponding critical spatial anisotropy $\gamma = J_i^z/J_i^{2z}$ is shown in Fig. 5. Because the frustration ratio $J_i^z/J_i^{2z}$ is highly tunable with pressure owing to the strong dependence of ferromagnetic couplings on the cation–anion–cation angle of the superexchange path$^{48}$, $S = 1/2$ frustrated magnets are promising candidates for realizing the Efimov effect without the strong exchange anisotropy. The same approach can also be applied to quasi-two-dimensional frustrated magnets$^{49}$.

So far multi-magnon bound states have been observed mostly in quasi-one-dimensional compounds but with different experimental techniques, such as absorption spectroscopy$^{12,15,17}$, inelastic neutron scattering$^{13,14,16,19,20,22,23}$ and electron spin resonance$^{43}$. The same spectroscopic measurements can be used here to observe the emergent Efimov states of magnons, provided that the conservation of the magnetization along the magnetic field axis is weakly violated$^{8,9,20}$. We found that even the lowest bound state of three magnons is already consistent with the universal Efimov state. Its binding energy for ferromagnetic cases is $5 \sim 55\%$ of the exchange coupling, which can be up to $10^7 \sim 10^9$ K. As a dilution refrigerator can lower the temperature down to a few tens of millikelvin, the observation of the lowest one or Efimov state(s) is within reach.

**Methods**

Two-magnon problem. The Schrödinger equation (3) for two magnons ($N = 2$) can be solved in a standard way. By treating the first term in the right hand side as a free part ($H_0$) and the rest as an interaction part ($V$), the two-magnon Schrödinger equation can be brought into the Lippmann–Schwinger equation:

$$\psi_2(\rho) = \phi_2(\rho) + \frac{1}{E - H_0 + i0^+} V |\psi_2\rangle$$

$$= \phi_2(\rho) + \int_{\gamma=0}^{\gamma=\pi} \frac{dk}{2\pi} \frac{\cos(k \cdot \rho)}{E - E(k) + i0^+} \times \left[ \sum_{J} \left( \cos \left( \frac{K}{2} \cdot \rho \right) - J_z \cos \left( \frac{k_i + k_i - K}{2} \cdot \rho \right) \right) \phi_2(\rho_k) - 2 D \phi_2(0) \right]$$

Here $\phi_2(\rho)$ is a solution to $E_h \phi_2(\rho) = H_0 \phi_2(\rho)$ and $E_0(k) \equiv E_0(\left(K/2 + k\right) + E_0(\left(K/2 - k\right) - k)$ is the energy of two non-interacting magnons. By setting $\rho = k, \rho = 0$ in equation (7), we obtain four coupled equations which determine the four unknown constants; $\psi_2(\rho_k)$ and $\psi_2(0)$, which in turn determine $\psi_2(\rho)$ through equation (7). The same result was obtained in the isotropic case of $I_z = 1$ and $D = 0$ in the pioneering work$^{48}$.

Three-magnon problem. The Schrödinger equation (3) for three magnons ($N = 3$) can be solved in a similar way. By treating the first term in the right hand side as a free part ($H_0$) and the rest as an interaction part ($V$), the Lippmann–Schwinger equation for $E < 0$ is written as

$$\Psi(r_1, r_2, r_3) = (r_1, r_2, r_3)| \frac{1}{E - H_0} V |\Psi\rangle$$

We then introduce a new parametrization of the wave function:

$$\chi_k(\rho; k) = \delta_{\rho, r_3} e^{-i(K - k) \cdot \rho} + r \psi(\rho; r_1, r_2, r_3)$$

which describes three magnons with a centre-of-mass momentum $K$ in which two of them are separated by a distance $\rho$ and the third one has a momentum $k$. The Bose statistics of magnons implies $\chi_k(\rho; k) = \chi_k(-\rho)$.

After a straightforward calculation, the Lippmann–Schwinger equation (8) can be brought into

$$\chi_k(\rho; k) = \int_{\gamma = \pi}^{\gamma = 0} \frac{dk}{2\pi} \frac{\cos \left( \frac{2k + k_i - K \cdot \rho}{2} \right)}{E - E_0(k_i, K - k_i - k, k_i)}$$

$$\times \left[ \sum_{J} \left( \cos \left( \frac{K - k_i}{2} \cdot \rho \right) - J_z \cos \left( \frac{k_i + k_i - K}{2} \cdot \rho \right) \right) \chi_k(\epsilon) \right]$$

$$+ 2 \sum_{J} \left( \cos \left( \frac{K - k_i}{2} \cdot \rho \right) - J_z \cos \left( \frac{k_i + k_i - K}{2} \cdot \rho \right) \right)$$

$$\times \chi_k(\epsilon) \left( -2 D \chi_k(0; k) - 4 D \chi_k(0; k) \right)$$

(9)
where $E_n(k, k, k') = \sum_{i=1}^{n} E_i(k_i)$ is the energy of three non-interacting magnons. By setting $\rho = \mathbf{x}, \mathbf{y}, \mathbf{z}$ and $\rho = 0$ in equation (9), we obtain four coupled integral equations which determine the allowed binding energy $E < 0$ and the four spin functions $\chi_{\mathbf{k}}(\mathbf{k}, \mathbf{k}, \mathbf{k})$ and $\delta_{\mathbf{k}}(\mathbf{k}, \mathbf{k})$, which in turn determine $\chi_{\mathbf{k}}(\mathbf{p}; \mathbf{q})$ through equation (9).

Bound-state solutions in the s-wave channel at $K = 0$ correspond to those where $\chi_{\mathbf{k}}(\mathbf{k}, \mathbf{k}, \mathbf{k}, \mathbf{k}) = \sum_{i=n}^{n} \delta_{\mathbf{k}}(\mathbf{k}, \mathbf{k}) = \delta_{\mathbf{k}}(\mathbf{k}, \mathbf{k}, \mathbf{k}, \mathbf{k}) = \delta_{\mathbf{k}}(\mathbf{k}, \mathbf{k}, \mathbf{k}, \mathbf{k})$, which is symmetric under any exchange among $\mathbf{k}, \mathbf{k}, \mathbf{k}, \mathbf{k}$, and all of them are even functions of $\mathbf{x}, \mathbf{y}, \mathbf{z}$.

The resulting two coupled integral equations with three variables ranging from 0 to $\pi$ are solved numerically by discretizing each variable with the Gaussian quadrature rule.

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