Letter

A distinguishable single excited-impurity in a Bose–Einstein condensate

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Abstract

We investigate the properties of a distinguishable single excited state impurity pinned in the center of a trapped Bose–Einstein condensate in a one-dimensional harmonic trapping potential by changing the bare mass of the impurity and its interspecies interaction strength with the Bose–Einstein condensate. We model our system by using two coupled differential equations for the condensate and the single excited-impurity wave function, which we solve numerically. For equilibrium, we find that an excited-impurity induces two bumps or dips on the condensate for the attractive- or repulsive-interspecies coupling strengths, respectively. Afterwards, we show that the excited-impurity induced imprint upon the condensate wave function remains present during a time-of-flight expansion after having switched off the harmonic confinement. We also investigate shock-waves or gray-solitons by switching off the interspecies coupling strength in the presence of harmonic trapping potential. During this process, we found that the generation of gray bi-soliton or gray quad-solitons (four-solitons) depend on the bare mass of the excited-impurity in a harmonic trap.

Keywords: Bose–Einstein condensate, impurity, solitons

(Some figures may appear in colour only in the online journal)

1. Introduction

Certainly, the physics of trapped condensates has emerged as one of the most exciting fields of physics in the last few decades. During the last few years, substantial experimental and theoretical progress has been made in the study of the properties of this new state of matter. The remarkable experimental realization of a Bose–Einstein condensate mixture composed of two spin states of $^{87}$Rb [1, 2] promotes a compelling interest in the physics of a new class of quantum fluids: the two or more species Bose–Einstein condensates [3–6]. Multi-species condensates (MSC) offer new degrees of freedom, which give rise to a rich set of new issues [7, 8]. At the heart of many of these issues is the presence of interspecies interactions and the resulting coupling of the two condensates. Previous theoretical treatments have shown that due to interspecies interactions, the ground state density distribution of MSC can display novel structures that do not exist in a one-species condensate [9, 10]. The investigation of a hybrid system requires progress on several different fronts. For example, in the last few decades many theoretical and experimental researchers have focused on single-particle impurity control in a many-body system for the detection and engineering of strongly correlated quantum states [11–16].

Individually controllable impurities in a quantum gas grants access to a huge number of proposed novel applications [17–20]. In the direction of quantum information processing, atomtronics applications are envisioned with single atoms acting as switches for a macroscopic system in an atomtronics circuit [21], two impurity atoms immersed in a quantum gas can be employed for a transfer of quantum information between the atoms [22], or individual qubits can be cooled preserving the internal state of coherence [23, 24]. Adding impurities and, hence, polarons one by one, allows
experimentally to track the transition even to the many-body regime and, moreover, yield information about spatial cluster formation [25–28]. Furthermore, adding single impurities one by one to an initially integrable system, such as a quasi one-dimensional Bose gas [29], allows one to controllably induce the thermalization of a non equilibrium quantum state. The coupling of impurities with condensed matter helps one to understand material properties such as molecule formation and electrical conductivity [30–34].

Recently, we investigated the static and dynamical properties of a single ground state impurity $^{133}$Cs in the center of a trapped $^{87}$Rb Bose–Einstein condensate (BEC) [35]. We studied the physical similarities and differences of bright shock waves and gray/dark bi-solitons, which emerge for an initial negative and positive interspecies coupling constant, respectively [35]. In this letter, we want to extend our previous work to the single excited impurity in the center of a trapped BEC. In section 2, we define two coupled one-dimensional differential equations, where one equation is nothing but a quasi one-dimensional Gross–Pitaevskii equation with a potential term stemming from the excited-impurity, and the second equation is a typical Schrödinger wave equation with an additional potential originating from the BEC. Afterwards, we show that the single excited state impurity (SESI) imprint upon the condensate wave function strongly depends upon whether the effective SESI-BEC coupling strength is attractive or repulsive. Subsequently, the dynamics of the SESI imprint upon the condensate wave function is discussed in detail in section 3. Here, we notice that for an attractive interspecies coupling strength the excited-impurity imprint does not decay but decreases for a repulsive interspecies coupling strength in a time-of-flight. In the same section 3, we discuss the creation of shock-waves or gray quad-solitons in a harmonic trap by switching off the attractive or repulsive Rb–Cs coupling strength. Finally, in section 4 we make concluding remarks and comment on the realization of the proposed model system.

2. Model

We assume an effective quasi one-dimensional setting with $\omega_z \ll \omega_I$, so the theoretical model for describing the time evolution of two-component BECs is the following coupled GP equations as

$$\frac{i}{\hbar} \frac{\partial}{\partial t} \psi(z,t) = \left\{ -\frac{\hbar^2}{2m_B} \frac{\partial^2}{\partial z^2} + \frac{m\omega_I^2}{2} z^2 + G_{\text{B}} |\psi(z,t)|^2 \right\} \psi(z,t),$$

$$\frac{i}{\hbar} \frac{\partial}{\partial t} \psi_I(z,t) = \left\{ -\frac{\hbar^2}{2m_I} \frac{\partial^2}{\partial z^2} + \frac{m\omega_I^2}{2} z^2 + G_{\text{B}} |\psi(z,t)|^2 \right\} \times \psi_I(z,t),$$

(1)

(2)

where $\psi(z,t)$ denotes the macroscopic condensate wave function for the $^{87}$Rb BEC and $\psi_I(z,t)$ describes $^{133}$Cs single excited state impurity with $z$ being the spatial coordinate, here $m_B$ and $m_I$ stand for the mass of the $^{87}$Rb and $^{133}$Cs atom, respectively. In the above equation (1), $G_{\text{B}} = 2N_B a_B \hbar \omega_I$ represents the one-dimensional $^{87}$Rb coupling strength, where $N_B = 200$ denotes the number of $^{87}$Rb atoms, and the $s$-wave scattering length is $a_B = 94.7 \ a_0$ with the Bohr radius $a_0$. In the first equation, $G_{\text{B}} = N^2_B \hbar$ stands for the impurity-BEC coupling where $g_{\text{B}} = 2a_B \hbar \sqrt{\omega_I} f(\omega_I/\omega_I)$ and $f(\omega_I/\omega_I) = (1 + (m_B/m_I)) / [1 + (m_B \omega_I) / (m_I \omega_I)]$ represents a geometric function [35], which depends on the ratio of the trap frequencies, and $N_B = 1$ stands for the number of excited-impurity atoms, and $a_B = 650 \ a_0$ expresses the effective Rb–Cs $s$-wave scattering, which can be modified by Feshbach resonance [31, 36–39]. Here $G_{\text{B}} = N_B g_{\text{B}}$ describes the BEC-impurity coupling strength. Presently, we show that the excited-impurity and the BEC are in the same trap, therefore, $\omega_I = \omega_I = 2\pi \times 0.179$ kHz and $\omega_B = \omega_B = 2\pi \times 0.050$ kHz. When the impurity atom decays to its ground state, it emits a photon with energy corresponding to the difference between the excited and ground states of a $^{133}$Cs atom. In our case, we show that the decay of the excited-impurity atom is damped by using the quantum zeno effect [40–42]. The quantum zeno effect is an aspect of quantum mechanics, where a particle’s wave function time evolution can be seized by measuring it frequently enough with respect to some chosen measurement setting. If the period between measurements is short enough, the wave function usually collapses back to the initial state [40–42]. In order to make equations (1) and (2) dimensionless, we establish the dimensionless coordinate as $z' = z/I_R$, the dimensionless time as $t' = \omega_I t$, and the dimensionless wave function as $\tilde{\psi} = \psi \sqrt{I_r} \tilde{\psi} = \psi \sqrt{I_r}$, where the oscillator length $l_r = \sqrt{\hbar / (m_B \omega_I)}$ is given by $28742.3 \ a_0$ for the above-mentioned experimental values. Therefore, equations (1) and (2) can be rewritten in dimensionless form

$$\frac{i}{\hbar} \frac{\partial}{\partial t'} \tilde{\psi}(z',t') = \left\{ -\frac{\hbar^2}{2} \frac{\partial^2}{\partial z'^2} + \tilde{\omega}_I^2 \tilde{\psi}(z',t')^2 + \tilde{G}_{\text{B}} \right\} \tilde{\psi}(z',t'),$$

$$\frac{i}{\hbar} \frac{\partial}{\partial t'} \tilde{\psi}_I(z',t') = \left\{ -\frac{\hbar^2}{2} \frac{\partial^2}{\partial z'^2} + \tilde{\omega}_I^2 \tilde{\psi}_I(z',t')^2 + \tilde{G}_{\text{B}} \tilde{\psi}(z',t')^2 \right\} \times \tilde{\psi}_I(z',t')$$

(3)

(4)

here, the first equation (3) describes the dynamics of the BEC, and the second equation illustrates the dynamics of the SESI. In the above equations, $\tilde{\alpha} = l_r/I_r$ has the value 0.808, here $\tilde{G}_{\text{B}} = 2N_B \omega_B a_B / \omega_I l_r$, and $\tilde{g}_{\text{B}} = 2a_B \omega_B f(\omega_B/\omega_I) / \omega_I l_r$ are the dimensionless Rb–Rb and Rb–Cs coupling strengths, respectively. By using these experimental values, we obtained the dimensionless Rb–Rb and Rb–Cs coupling strengths as $\tilde{G}_{\text{B}} = 4.71$ and $\tilde{g}_{\text{B}} = 0.16$, respectively. From here on, we will drop all the tildes for simplicity. To find the numerical excited state of a Cs impurity, we start with a trial excited state wave function for the impurity as summarized in appendix A; here the impurity dimensionless energy $\tilde{E}_1$ depends upon the dimensionless imaginary time.

In order to determine the equilibrium excited-impurity imprint on the condensate wave function, we solve numerically the two coupled dimensionless quasi one-dimensional Gross–Pitaevskii equation (3) for the BEC and the differential
equation (4) for the excited-impurity by using the split-operator method [43–46]. In this way, we demonstrate that the $^{133}$Cs excited-impurity leads to two bumps or two holes at the center of the $^{87}$Rb BEC density for attractive or repulsive interspecies coupling strength $g_{IB}$ as displayed in figures 1(a) and (b), respectively. For stronger attractive $g_{IB}$ values two bumps can increase further as depicted in figure 1(a), but for strong repulsive $g_{IB}$ values two dips in the BEC density get deeper and deeper until BEC fragments into three parts as illustrated in figure 1(b). Additionally, the SESI effective mass increases quadratically for interspecies coupling strength $g_{IB}$ as presented in appendix B. In this article, we have utilized the zero-temperature GP mean-field theory, however, as a matter-of-fact, elementary excitations can arise from the thermal and/or quantum fluctuations [47], and the BEC dynamics may be considerably affected by the motion of the excited atoms around it (thermal cloud), and by the dynamical BEC depletion [48]. To give a rough estimate, first of all, we show that the excited-impurity in our proposed model does not affect the mean-field description of our system. The mean-field approximations hold so long, as the impurity-BEC interaction does not significantly deplete the condensate, leading to the condition [49–51]

$$|a_{IB}|\xi^{-1} \ll 1.$$  \hspace{1cm} (5)

Here, $\xi^{-1} = l/\sqrt{2M_{1D}a_{IB}}$ is the 1D healing length. The dimensionless peak density of the BEC at the center of the condensate is $n_{1D} = 0.355(0.164)$ for the dimensionless Rb–Rb coupling strength $G_{B} = 10(100)$ and the corresponding value $|a_{IB}|\xi^{-1} = 0.0020(0.0014)$, respectively. Which shows that our treatment of the single excited-impurity in a BEC system neglects the phenomenology of strong-coupling physics, e.g. near a Feshbach resonance [52], which lies beyond the parameter range of equation (5). Therefore, we restrict the following calculation of the validity range of the mean-field analysis to a BEC without any excited-impurity. Additionally, in appendix C, we regulate how quantum and thermal fluctuations within the Bogoliubov theory restrict the validity range of our mean-field description.

3. Dynamics of the BEC and the excited-impurity

To investigate the dynamical evolution of the condensate wave function and the excited-impurity, we investigate numerically two quench scenarios. In the first scenario, we investigate the standard time-of-flight expansion after having switched off the external harmonic trap when the excited-impurity and BEC interspecies interaction strength is still present. In the second case, we consider an inverted situation where the excited-impurity and the BEC interspecies interaction strength is turned off by letting the harmonic confinement be switched on. This represents an interesting scheme to generate matter waves like shock-waves or solitons depending on whether the initial excited-impurity and BEC interaction strength is attractive or repulsive.

In the first scheme, we turn off the magnetic trap at time $t = 0$; the BEC and the SESI are allowed to expand in all directions. At $t = 0$, the confining potential vanishes, and further acceleration results from inter- and intra-species interactions strength. For the attractive or repulsive interspecies coupling strength, two bumps or dips decay slowly during the temporal evolution as shown in figures 2(a) and (d). The relative speed of decay of these bumps or dips from each other is zero. The SESI imprint bumps or dips are not only decaying but also moving away from their stationary positions as demonstrated in figures 2(c) and (f).

In the second scenario, we introduce a numerical model of matter-wave self-interference resulting from the attractive and repulsive interspecies strength being switched off and within a remaining harmonic confinement, which leads to shock waves and gray quad-solitons, respectively, as predicted in figures 3(a) and (c). We observed that in every scenario, approximately $t < 0.045$ dimensionless time is required to generate shock-waves or quad-solitons as shown in figures 3(a) and (c), respectively. For an initial attractive interspecies coupling strength $g_{IB} = -40$, we examine how two excitations of the condensate are generated at the SESI position that travel in different directions with identical center-of-mass speed, and are reflected at the harmonic confinement boundaries and then collide at the SESI position as depicted in figure 3(a). We have made different calculations by changing the value of $g_{IB} < 0$. In all cases we observed the appearance of shock wave structures as shown in figure 3(a). The density of depleted atoms around the shocks becomes, at most, larger than the depletion density far away from perturbations. The corresponding excited-impurity self-interference pattern starts breathing with dimensionless frequency $\omega_{f}/\omega_{x} = 2$ at the center of the harmonic trap as shown in figure 3(b). For small attractive/repulsive interspecies scattering strength the excited-impurity self-interference fringes show smaller strength as discussed in...
appendix D. We can determine the breathing frequency of the SESI in a harmonic trap by defining the single excited-impurity wave function
\[ \psi_I(z, t) = \sqrt{\frac{2}{\pi A(t)^3}} e^{-z^2/\pi A(t)^2 - i R(t)}, \]
here \( A(t) \) defines the dimensionless width of the SESI and \( R(t) = -A'(t)/2\alpha^2A(t) \) describes the variational parameter, which defines the momentum of the SESI. We write the equation of motion for the width of the excited-impurity by determining the Euler–Lagrangian equation of the system in
\[ A''(t) - \frac{\alpha^4}{A(t)^4} + A(t) = 0, \] (6)

where the equilibrium state is \( A(t=0) = A_0 = \alpha \) and \( \alpha = \hbar z / \hbar_s \) has the equilibrium value 0.808. We solve equation (6) and get the time dependent width of the excited-impurity

\[ A(t) = \sqrt{\frac{\alpha^4 + (A_0^4 - \alpha^4) \cos(2t) + A_0^4}{2A_0^4}}. \]

Thus, in order to get the excited-impurity out of equilibrium we can let \( A_0 = \alpha \pm \delta \), where \( \delta \) is a small quantity. From the time dependent width of the excited-impurity, we identify the dimensionless breathing oscillation frequency to be \( \omega_I / \omega_s = 2 \).

For the repulsive interspecies coupling strength \( g_{IB} = 80 \), we inspect gray quad-solitons, traveling with the same speed as shown in figure 3(c). In the case of harmonic confinement with a dimensionless potential \( V_{\text{ext}} = \frac{1}{2} \), the frequency of the oscillating soliton differs from the trap frequency by a factor \( \omega_1/\omega_s = 1/\sqrt{2} \), with a unique frequency \( \omega_1/\omega_s = 2 \) as shown in figure 3(d), which we calculated by solving equation (6). We also find that the excited-impurity density self-interference patterns do not pass through each other at \( z = 0 \), which is quite clear as they do not exhibit solitonic behavior as demonstrated in figures 3(b) and (d).

To illustrate a more general case for the generation of the solitons by pinning the excited-impurity in the center of the BEC, we investigate different masses’ impurities, which basically change nothing in our proposed model but the value of parameter \( \alpha = \sqrt{m_I/m_B} \). For the value of \( \alpha = 0.2 \), we witness a new kind of phenomena where only two gray-solitons are generated as the distance between the maxima
and the minima of the excited-impurity wave function is quite small; therefore solitons get the overall shape of the sculpted BEC as depicted in figure 4(a). The shape of these gray bi-solitons is totally different than the shape of the solitons for parameter $\alpha = 0.808$, as demonstrated in figure 3(c). For the case $\alpha = 0.2$ near to the trap boundary, the solitons do not attract each other, as they express united identity, as demonstrated in figure 4(a). Additionally, these bi-solitons oscillate in a harmonic trap with the same dimensionless frequency $\omega_s/\omega_z = 1/\sqrt{2}$ as predicted in the previous case. In figure 4(d), we use $\alpha = 1.5$, in this scenario, again quad gray-solitons are generated, which reveal similar properties as discussed for the case of $\alpha = 0.808$. Furthermore, the SESI interference fringes’ height decreases with increasing the bare mass of the excited-impurity and vice versa as demonstrated in figures 4(c) and (f). However, we observe that the number of interference fringes increases with increasing the bare mass of the excited-impurity as illustrated in figures 4(c) and (f). Additionally, as the bare mass of the SESI increases, the width of the center-of-mass of the solitons decreases, as shown in figures 4(a) and (d). The reason for this is quite simple and clear, as the solitons depth increases with increasing mass, they can not move away from their central position.

4. Discussion

Our studies elucidate the role of a single excited state impurity pinned in a $^{87}$Rb BEC. We model our system in the mean-field regime by writing the one-dimensional two coupled differential equations. This approximation is valid for relatively weak interspecies interaction and for single excited-impurity. We pinned the excited-impurity in the condensate center and diminished its decay by using the quantum zeno effect. We found that the BEC depletion induced by the single excited state impurity causes the BEC density to split into three parts. During our calculations, we found that the excited-impurity imprint decays marginally for the attractive interspecies coupling strength; and in repulsive interspecies coupling strength, it starts to decay significantly as compared to the small value of the interspecies interaction strength. We have used a numerical simulation to analyze the generation and dynamics of gray quad-solitons or bi-solitons in the Bose–Einstein condensate. We disclose that the shape of newly generated solitons depends on the bare mass of the excited state impurity. We would like to remark that even though in our analysis we use an idealized potential for the excited-impurity, such an approximation is known to not only encapsulate the basic physics, but can also be a good approximation to experimental setups.

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specific dimensionless imaginary time interval which later decays to its ground state, as shown in figure A1.

Appendix B. Effective mass

The effective mass of the excited-impurity is denoted as \( m_{\text{eff}} = \frac{\hbar}{(l_{\text{Iz}}^2 \omega_z)} \), where the excited-impurity oscillator length \( l_{\text{Iz}} = \sqrt{2} \sigma \) comes from the standard deviation \( \sigma = \sqrt{<z^2> - <z>^2} \), with \(<\bullet> = \int \psi(z)^* \psi(z) dz\) representing the expectation value. Figure A2 shows the ratio of the effective mass of the \(^{133}\text{Cs}\) impurity with respect to the bare mass \( m_{\text{I}} \), which increases quadratically for interspecies coupling strength \( -10 < g_{\text{IB}} < 10 \), as shown in the inset of figure A2, and becomes marginally saturated for interspecies coupling strength \( g_{\text{IB}} > 80 \). Here, we utilize the mean-field regime to determine the effective mass of the excited-impurity. Through this connection, one may extend this work to investigate polaron physics, in order to include the impact of quantum and thermal fluctuations [26, 27, 60, 61].

Appendix C. Mean-field analysis

To give a rough estimate, first of all we show that the excited-impurity in our proposed model does not affect the mean-field description of our system. Therefore, we restrict the following calculation of the validity range of the mean-field analysis to a BEC without any excited-impurity. In the following, we regulate how quantum and thermal fluctuations within the Bogoliubov theory restrict the validity range of our mean-field description.

C.1. Quantum depletion

According to the Bogoliubov theory the three-dimensional quantum fluctuation term is defined in the Thomas–Fermi approximation:

\[
\begin{align*}
\mathcal{N}_{\text{QF}} \left( \mathbf{r} \right) &= \mathcal{N}^0_{\text{B}} \left( \mathbf{r} \right) - \mathcal{N}_B \left( \mathbf{r} \right) = \frac{8}{3\sqrt{\pi}} \left[ N_B \alpha_B \mathcal{N}^0_{\text{B}} \left( \mathbf{r} \right) \right]^{3/2}. \quad \text{(C.1)}
\end{align*}
\]

We assume an effective one-dimensional setting with \( \omega_z \ll \omega_r \), so we decompose the BEC wave-function \( \psi_B(\mathbf{r}, t) = \psi_B(z, t) \phi_B(\mathbf{r}_\perp, t) \) with \( \mathbf{r}_\perp = (x, y) \) and

\[
\phi_B(\mathbf{r}_\perp, t) = e^{-\frac{x^2 + y^2}{m_B \omega_r^2}} e^{-i \mathbf{k}_r \mathbf{r}_\perp t}. \quad \text{(C.2)}
\]

We integrate out the transversal degrees of freedom from equation (C.1) to get an effective one-dimensional setting

\[
\begin{align*}
\mathcal{N}_{\text{QF}}^\text{ID} \left( z \right) &= \mathcal{N}_{\text{QF}} \left( \mathbf{r} \right) = \frac{16}{9\pi \omega_r} \left[ N_B \alpha_B \mathcal{N}^0_{\text{B}} \left( z \right) \right]^{3/2}. \quad \text{(C.3)}
\end{align*}
\]

We know that for larger inter-particle interaction strength the BEC density is characterized by the Thomas-Fermi (TF) profile \( \mathcal{N}_B^\text{ID}(z) = \frac{\mu_B^\text{ID}}{\mu_B} \left( 1 - \frac{z^2}{R_f^2} \right) \) with \( R_f^2 = \frac{\mu_B^\text{ID}}{\hbar^2 m_B \omega_r^2} \). With this we
calculate the one-dimensional quantum fluctuation depleted term with respect to the number of particles $N_B = 200$ by using $N_{QF}^{ID} = \int n_{QF}^{ID}(z)dz$ and get
\[
N_{QF}^{ID} = \frac{3}{4} \left( \frac{a_B^2 N_B}{\sqrt{2}} \right)^{1/3}.
\] (C.4)
We evaluate this relative depletion for the system parameters of our study. With this we obtain from (C.4) $\frac{N_{QF}}{N_B} = 0.0022$, so that the quantum fluctuations are, indeed, negligible.

C.2. Thermal depletion
Correspondingly, the one-dimensional thermal depleted term with respect to the number of particles follows from the Bogoliubov theory to be
\[
N_{TF}^{ID} = \gamma \left( \frac{T}{T_c} \right)^2
\] (C.5)
with the dimensionless prefactor
\[
\gamma = \frac{5^{2/5} \pi^2}{2^{3/5} \times 3^{3/5}} \frac{N_{TF}^{ID}}{N_B} \left( \frac{N_B}{\xi (3)^{8/3} T_c^2 l_c^{1/3}} \right)^{1/5}.
\] (C.6)
For our system parameters we obtain $\gamma = 0.046$ and the critical temperature $T_c = \frac{\hbar}{k_B} \left( \omega^2 \omega_c^2 N_B \right)^{1/3} = 14.7$ nK. Thus, choosing a reasonable ratio of the thermal depleted term $\frac{N_{TF}^{ID}}{N_B} = 0.001$, we estimate the temperature of the system to be
\[
T = T_c \sqrt{\frac{1}{\gamma} \frac{N_{TF}^{ID}}{N_B}} = 2.15 \text{ nK}.
\] (C.7)
With this we conclude that if the temperature of the system is lower than $T = 2.15 \text{ nK}$, the thermal fluctuations are not affecting the Bose–Einstein condensate.

Appendix D. Excited-impurity self-interference patterns
The single excited-impurity wave packet displays self-interference patterns as shown in figure A3. The excited-impurity wave function has one maxima and one minima, therefore when the attractive/repulsive interspecies coupling strengths are switched off, then the excited-impurity self-interference patterns are generated. We find that the excited-impurity density self interference patterns do not pass through each other at $z = 0$, which is quite clear as they do not exhibit solitonic behavior, as shown in figure A3. As can be seen in figure A3, for small attractive/repulsive interspecies scattering strength the excited-impurity self-interference fringes demonstrate smaller strength and vice versa.

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