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Soliton Molecules in the Impurity Component of Self-Trapping Bosonic Impurity

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Abstract: We investigate the dynamics of soliton molecules in the impurity component of a trapped Bose-Einstein condensate-impurity mixture (polaronic soliton molecules) using the time dependent Hartree-Fock-Bogoliubov equations in a quasi one-dimensional geometry. We show that the impurity component which obeys the self-focussing nonlinear Schrödinger equation, supports bright soliton molecules even for repulsive interspecies interactions. The binding energy, the width, the equilibrium state and the evolution of such solitons are deeply analyzed within variational and numerical means. We find that our variational and numerical calculations well coincide with each other.

Keywords: Soliton-Molecules, Impurity, BEC, NLSE

1. Introduction

Bose-Einstein condensate (BEC)-impurity mixture known as Bose polaron problem, has attracted considerable attention at the frontier of condensed matter both theoretically and experimentally [1-16].

During the last decades, intensive theoretical and experimental works have been devoted to the existence, stability and the dynamics of solitons. Such localized nonlinear excitations structures have been identified as critical components of numerous continuous and discrete dynamical systems. Solitons are indeed, ubiquitous in nature due to their experimental realization in many diverse systems including, but not limited to, optical fibers, waveguide arrays, photonic crystals, BECs, molecular crystals, quasi one-dimensional (1D) solids, Josephson-junctions, layered silicates, micromechanical cantilever arrays, pendulum arrays, water waves, electrical transmission lines, ferromagnetic and antiferromagnetic materials, granular crystals and so on. Additionally, they play an important role in denaturation transitions and bubble formation in DNA, protein folding, atom ejection and defect migration in crystals, and many others systems.

Recently, solitons in Bose polaron systems have gained immense interest in the field of ultracold atoms [10, 13, 17]. Indeed, polaronic soliton is a bit different to the ordinary one. How? When an impurity is immersed in a BEC, it can spontaneously form a self-localized state. In the strong coupling limit, this localized state exhibits a solitonic behavior in a quasi-1D geometry. These embedded solitons inside the condensate may remain robust during its evolution if (i) the condensate preserves its form (i.e. does not decay) and (ii) the impurity-condensate interaction is weak. Furthermore, impurity solitons decay with rising temperature and in the case of strong host-host and impurity-host interactions. They can also split into several picks forming a soliton train when the pairing instability (anomalous correlation) is suddenly increased [13]. Quite recently, the properties of polaronic two-soliton molecules and vector solitons of a trapped BEC-impurity mixture subjected to a PT-symmetric potential in a quasi-1D setup have been investigated analytically and numerically by one of us [18].

Recently, a stable bound state of three solitons in dispersion-managed optical fibers was realized experimentally [19, 20] and confirmed theoretically [21-23]. The main motivation behind creating such molecules is to increase the bit-rate of data transfer in optical fibers beyond the binary regime.

In view of these circumstances it is therefore, interesting to check the existence of three-soliton molecules in Bose polaron systems. The study of polaronic solitons is a long-standing challenge for research in fundamental and applied science, due to their importance in understanding and

predicting phenomena arising in both nonlinear and condensed matter systems.

The goal of this paper is to study the dynamical properties of Bose polaronic three-soliton molecules in a quasi-1D geometry employing our time dependent Hartree-Fock-Bogoliubov (TDHFB) model [13, 14, 17, 24-29]. The TDHFB theory is a set of coupled nonlinear equations of motion for the condensate, thermal cloud, anomalous density (pairing state) and the impurity. It is a natural extension of the Gross-Pitaevskii equation that is valid only at zero temperature. The TDHFB approach constitutes an efficient tool to investigate the properties of impurity solitons in any interaction and temperature regime. By means of a variational approximation and a numerical simulation, we analyze the stability and the binding mechanism of three solitons. In most cases, the variational method provides good accuracy and correctly predicts the numerical results. The dynamics of such structures will also be studied using an appropriate numerical scheme.

The practical implementation of our approach requires extensive research on the stability domains, mutual interactions and propagation dynamics of soliton molecules in Bose polaron system. One should stress at this stage that the stability of three solitons is not an easy task due to the inherent repulsive force between adjacent solitons.

The rest of paper is organized as follows. In Sec. 2, we review the main steps of our formalism and subedit the problem. Section 3 is devoted to develop the variational model. To this end, we choose a trial function that is able to capture the main physics of the problem at hand. In Sec. 4, we perform our numerical simulations. In Sec. 5, we draw our concluding remarks.

2. Formalism

This section introduces the TDHFB theory for Bose polaron problems.

We consider a mobile impurity of mass m_I immersed in a BEC of atoms of mass m_B at finite temperature. The impurity-boson interaction and host-host interactions have been approximated by the contact potentials $g_B\delta(r-r')$ and $g_{IB}\delta(r-r')$, respectively. The TDHFB equations describing the dynamics of the condensate, thermal cloud, the anomalous density and the impurity read [13, 14, 17]

$$i\hbar\dot{\Phi}_B = \left[h_B^{sp} + g_B\left((\beta-\dot{2})n_B + 2n + \gamma n_I\right)\right]\Phi_B, \quad (1)$$

$$i\hbar\dot{\tilde{m}} = 4\left[h_B^{sp} + g_B(2G\tilde{m} + 2n + \gamma n_I)\right]\tilde{m}, \quad (2)$$

$$i\hbar\dot{\Phi}_I = \left[h_I^{sp} + g_{IB}(n_B + \tilde{n})\right]\Phi_I. \quad (3)$$

In Eqs. (1)-(3), $h_B^{sp} = -(\hbar^2/2m_B)\Delta + V_B$ and $h_I^{sp} = -(\hbar^2/2m_I)\Delta + V_I$ are, respectively the single particle Hamiltonian for the condensate and the impurity. $\Phi_B(r) = \langle\hat{\psi}_B(r)\rangle$ is the condensate wave function, $n_B(r) = |\Phi_B(r)|^2$ is the condensed density, $\Phi_I(r) = \langle\hat{\psi}_I(r)\rangle$ is the impurity wave function, $n_I(r) = |\Phi_I(r)|^2$ is the density of impurity atoms, the noncondensed density $\tilde{n}(r)$ and the anomalous density $\tilde{m}(r)$ are identified, respectively with $\langle\hat{\psi}^+(r)\hat{\psi}(r)\rangle - \Phi_B^*(r)\Phi_B(r)$ and $\langle\hat{\psi}(r)\hat{\psi}(r)\rangle - \Phi_B(r)\Phi_B(r)$, where $\hat{\psi}^+$and $\hat{\psi}$ are the boson destruction and creation field operators, respectively. The total density in BEC is defined by $n = n_B + \tilde{n}$. The dimensionless parameters $\beta = U/g_B$ with $U = g_B(1 + \tilde{m}/\Phi_B^2)$ being the renormalized coupling constant [27], $G = \beta/4(\beta-1)$ and $\gamma = g_{IB}/g_B$is the relative coupling strength.

Note that Eqs.(1) can also be used to study vector solitons such as bright-bright-bright, bright-bright-dark or dark-dark-bright solitons,… producing in the whole mixture when fields of the impurity and its bath are combined [13].

Under the weak impurity-boson coupling assumption, the condensate and the anomalous density are in the Thomas-Fermi regime i.e. the kinetic terms in Eqs. (1a) and (1b) are negligible. Replacing the resulting equations in Eq. (1c), we find that Φ_I obeys the generalized self- focusing nonlinear Schrödinger equation (NLSE)

$$i\hbar\dot{\Phi}_I = \left(\left(-\frac{\hbar^2}{2m_I}\right)\Delta + V_I - \lambda V_B - \upsilon_I - \mu_I - g_B\gamma\lambda n_I\right) = \Phi_I, \quad (4)$$

where $\lambda = \gamma[1/(\beta-2) + 1/2G]$ and $\upsilon_I = (2ng_B - \mu_B)\lambda$. For $\beta = 1$, Eq.(4) is nothing else than the standard NLSE.

It is clearly seen from Eq.(4) that even we assume the forces between atoms in a pure Bose component to be effectively repulsive, their character can be changed from repulsive to attractive in the presence of an impurity provided the BEC and impurity attract each other strongly enough. Therefore, in such a regime the impurity component becomes a system of effectively attractive atoms leading automatically to the generation of bright solitons.

Indeed, the change in the sign of the interaction parameter λ affects also the form of the solitonic solution. For instance, for $\beta > 2$, $\bar{g} > 0$, λ is positive and thus, the impurity wave packet has an attractive interaction between atoms, so that the system supports automatically bright solitons. Whereas, for $1 < \beta < 2$, λ is negative and hence, the impurity behaves as a dark soliton. Remarkably, the λ has a minimum at certain critical value $\beta = 6.83$. The whole behavior of the parameter λ as a function of β is displayed in figure 1.

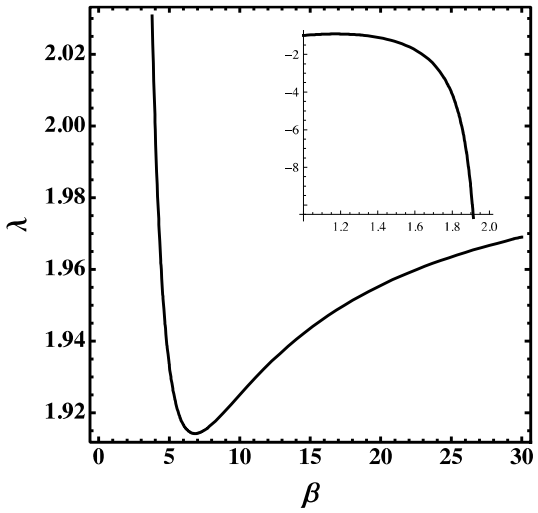

Figure 1. *Interaction parameter λ as a function of β.*

In what follows, we consider an impurity embedded in a BEC confined in highly anisotropic trap where the longitudinal and transverse trapping frequencies are $\omega_{Bx}/\omega_{B\perp} \ll 1$. In such a case, the system can be considered as quasi-1D. Therefore, the coupling constants take their 1D form, namely $g_B = 2\hbar\omega_{B\perp}a_B$ and $g_{IB} = 2\hbar\omega_{B\perp}a_{IB}$, where a_B and a_{IB} are the scattering lengths describing the low energy boson-boson and impurity-boson scattering processes.

It is convenient to rewrite Eq.(4) in terms of dimensionless quantities using the following parameters: $x = x/l_I$ where $l_I = \sqrt{\hbar/m_I\omega_I}$ is the impurity oscillator length, $\alpha = m_B/m_I$ is the ratio mass, $\Omega_\perp = \omega_{B\perp}/\omega_{I\perp}$, with $\omega_{I\perp}$ being the transverse impurity confinement frequency, $\tau = t\omega_{I\perp}$ and $\Phi_I = \Phi_I l_I^{1/2}$, we then get

$$i\frac{d\Phi_I}{d\tau} = \left(-\frac{1}{2}\Delta_x + \frac{1}{2}\varrho^2 x^2 - \bar{\upsilon_I} - \bar{g}n_I\right)\Phi_I, \tag{5}$$

where $\varrho^2 = 1 - \lambda\alpha\Omega_\perp^2$, $\bar{\upsilon_I} = \upsilon_I/\hbar\omega_{I\perp}$ and

$$\bar{g} = 2\lambda\Omega_\perp(a_{IB}/l_I).$$

The energy functional corresponding to the NLSE (5) reads

$$E = \int_{-\infty}^{\infty}\left(\frac{1}{2}|\nabla\Phi_I|^2 + \left(\frac{1}{2}\varrho^2 x^2 - \upsilon_{\mathrm{I}}\right)|\Phi_I|^2 - \frac{\bar{g}}{2}|\Phi_I|^4\right)dx. \tag{6}$$

The behavior of the energy of three solitons will be shown in the next section. Note that the energy (6) allows us to calculate the chemical potential of the molecule.

3. Variational Method

We restrict ourselves in this section to analyzing the formation of soliton-molecule (bound state of two or more solions) in the impurity component of a trapped BEC impurity mixture.

Let us now reveal the role of the impurity on the formation and on the stability of two (dimer) and three (trimer) bright soliton molecules. In the trapped case, Eq. (5) is not integrable since the integrability requires that ϱ and $\bar{g}$ to be time dependent. Therefore, to solve (5), we use a variational method. This latter is proved to be efficient for the analysis of non-integrable solitons in different domains of nonlinear physics. Below we develop our variational scheme for three-soliton molecules in the impurity component, using the following trial ansatz:

$$\Phi_I(x,t) = N\sum_{j=1}^{3}\exp\left[-\frac{(x-\eta_j)^2}{q_s^2} + i\phi_j\right], \tag{7}$$

where N guarantees the normalization of Φ_I to the number of solitons in the molecule, namely $N = 3$. The variational parameters $q_s(t)$, $\phi(t)$ and $\eta(t)$ correspond respectively to the width, the phase, and the peak position of the soliton.

Inserting the trial function (7) into Eq.(6), the energy of the single-soliton takes the form

$$E_1 = \frac{1}{2}\varrho^2\left(\frac{q_s^2}{2} + \eta_1^2\right) - \frac{\bar{g}}{2\sqrt{2\pi}q_s} + \frac{1}{4q_s^2} - \bar{\upsilon}, \tag{8}$$

whereas, the energy of two-soliton molecule is given by

$$E_2 = \frac{\Lambda_2}{2q_s^4\Lambda_1} + \frac{\varrho^2\Lambda_3}{8\Lambda_1} - \frac{\bar{g}\,\Lambda_4}{4\sqrt{\pi}q_s\Lambda_1^2} - \bar{\upsilon}, \tag{9}$$

where

$$\Lambda_1 = e^{\frac{(\eta_1-\eta_2)^2}{q_s^2}} + \sqrt{e^{\frac{(\eta_1-\eta_2)^2}{q_s^2}}}\cos(\phi_1-\phi_2),$$

$$\Lambda_2 = q_s^2 e^{\frac{(\eta_1-\eta_2)^2}{q_S^2}} + e^{\frac{(\eta_1-\eta_2)^2}{2q_S^2}}(q_s+\eta_1-\eta_2)(q_s-\eta_1+\eta_2)\cos(\phi_1-\phi_2),$$

$$\Lambda_3 = e^{-\frac{2\eta_1\eta_2}{q_S^2}}\left[e^{\frac{\eta_1\eta_2}{q_S^2}}\sqrt{e^{\frac{\eta_1^2+\eta_2^2}{q_S^2}}}\left(q_s^2 + (\eta_1+\eta_2)^2\cos(\phi_1-\phi_2) + e^{\frac{\eta_1^2-\eta_2^2}{q_S^2}}\left(q_s^2 + 2(\eta_1^2+\eta_2^2)\right)\right)\right],$$

$$\Lambda_4 = e^{\frac{\eta_1^2-4\eta_1\eta_2+\eta_2^2}{q_S^2}}\left[e^{\frac{\eta_1^2+6\eta_1\eta_2+\eta_2^2}{q_S^2}}\cos(\phi_1-\phi_2) + e^{\frac{\eta_1^2+\eta_2^2}{q_S^2}} + 2e^{\frac{2\eta_1\eta_2}{q_S^2}}\cos^2(\phi_1-\phi_2) + e^{\frac{2\eta_1\eta_2}{q_S^2}}\right].$$

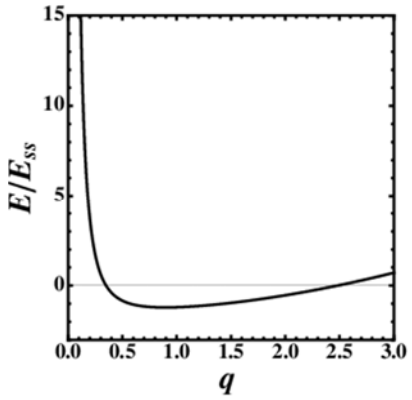

Figure 2. *Binding energy of two solitons relative to that of the single soliton energy E_{ss} as function of the width for $\beta = 2.5$, $\Omega = 1$, $\eta_1 = -\eta_2 = 0.5$, $\phi_1 = 0$ and $\phi_2 = \pi$.*

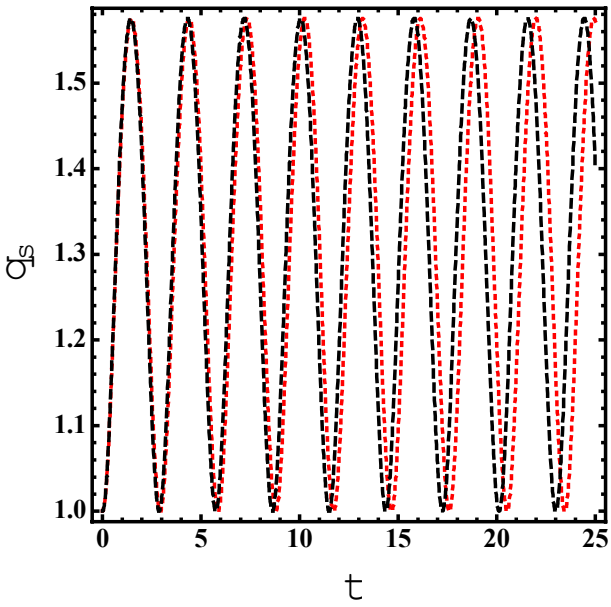

Figure 3. *Time evolution of the width of three solitons. Red dashed line: our numerical simulation of NLSE. Black solid line: our variational calculation: Parameters are the same as in figure 2.*

For the three soliton-molecule, the resulting energy that turns out to be lengthy and hence will not be shown here for convenience.

As is shown in figure 2, our variational calculation shows that three solitons display a pronounced local minimum indicating that these structures have nonzero binding energy and thus, have a molecular character. The depth of the minimum will give an estimate to the strength of the bond in the molecule. It is worth noticing that the bound state exists irrespective the presence of trapping potential or not [18, 21, 22].

Figure 3 shows that that the soliton width exhibits periodic oscillations during its time propagation. This can be attributed to the repulsive interactions between solitons. We see also from the same figure that the variational calculation coincides well with the numerical results.

4. Numerical Results

In order to check the validity of our variational calculation, we solve numerically the NLSE (5). The numerical simulations of two- and three-soliton molecules have been performed using the split-step fast Fourier transform method, which proved to be a powerful tool in solving a variety of nonlinear problems efficiently.

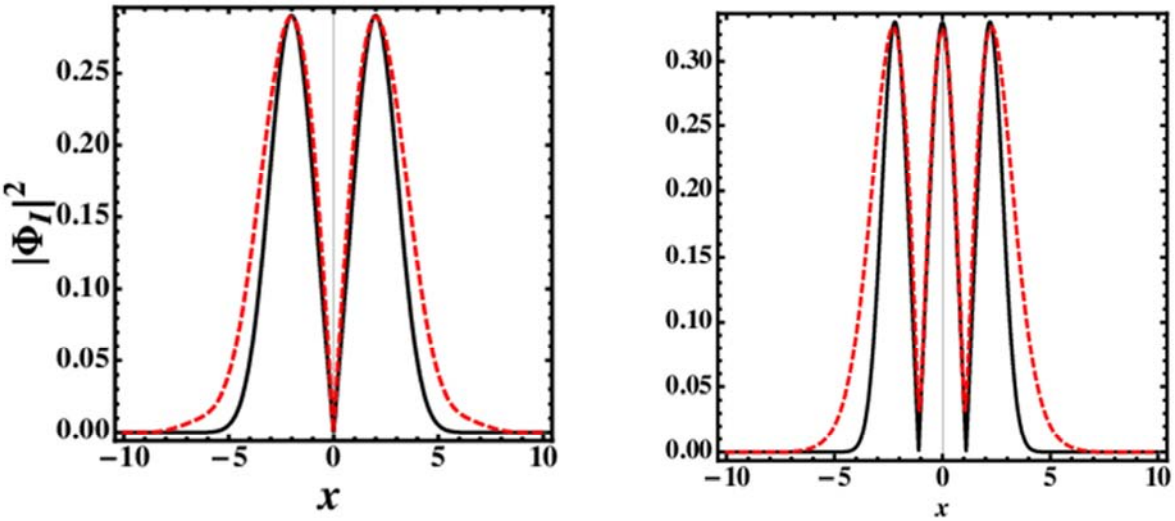

Figure 4. *(Color online) Density profile for the impurity two- and three soliton in BEC-Impurity system (left panel). Density profile for three-soliton molecule (right panel) with the same parameters as in figure (1). Red dashed line: numerical simulation of NLSE. Black solid line: variational calculation.*

In figure 4 we compare the soliton profiles obtained by our variational calculation with the simulation results of Eq. (5) for both two-soliton and three-soliton molecules. The figure shows the existence of robust two- and three-soliton molecules in a quasi-1D BEC-impurity system. Furthermore, as can be seen from the same figure that the variational calculation agrees well with the numerical simulation.

Figure 5 displays the time evolution of two-soliton molecule. We clearly observe that the two-soliton molecule remains almost stable during its time propagation. The fact that the molecule is stable this means that the two solitons placed at the equilibrium separation (distance in which the structure forms a stable soliton molecule). We then infer that our variational appraoch adequately describes the dynamics of the molecule close to the equilibrium state of solitons.

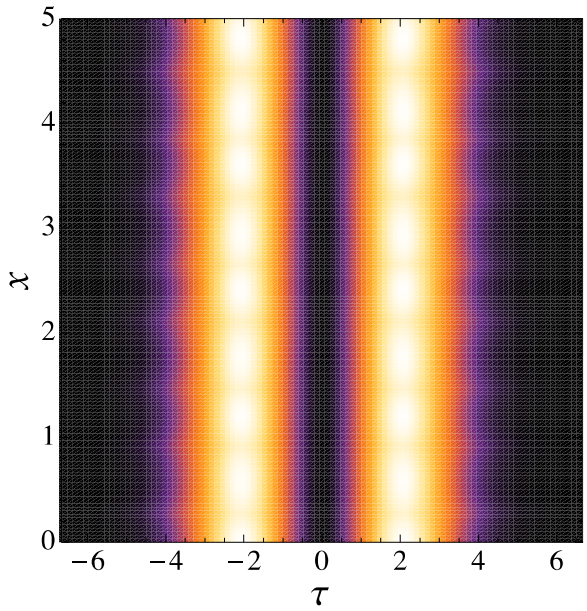

Figure 5. *(Color online) Spatio-temporal evolution of the shape of a two-soliton molecule, according to numerical solution of Eq. (4).*

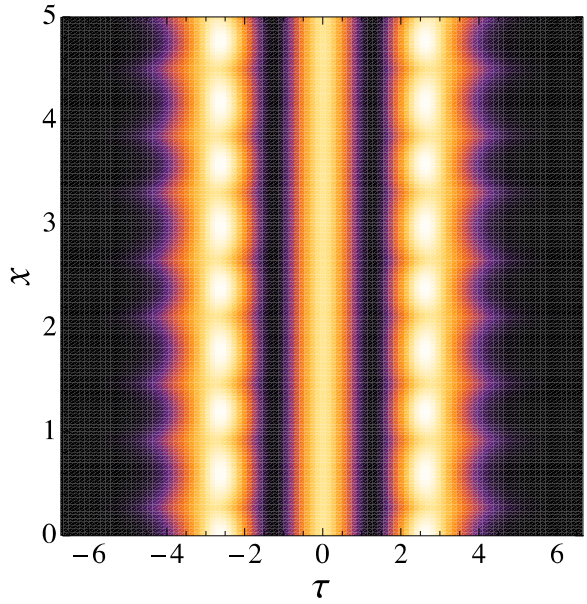

Figure 6. *(Color online) Spatio-temporal evolution of the shape of a three-soliton molecule. Parameters are the same as in figure 5.*

As is depicted in figure 6, the three-soliton molecule exhibits small oscillations during its evolution due to the immanent repulsive interactions between solitons. One can expect also that when solitons are placed at small inter-soliton separation, they periodically collide and repel each other. For very small distance, the three solitons merge and hence, the molecule disintegrates. While at large separations the solitons diverge and hence, do not interact anymore.

5. Conclusion

We have used the TDHFB equations to investigate analytically and numerically the dynamics of three-soliton molecules in the impurity component of BEC-impurity mixture. In the framework of the weak coupling regime, we have derived a self-focussing nonlinear equation governing the time evolution of soliton molecules in the impurity component. Employing a suitable variational ansatz, we have obtained useful analytical expressions for the binding energy of two and three solitons. We found that this energy has a local minimum indicating that such solitons form a molecule. We showed that the width exhibits periodic dynamics. Furthermore, we have solved numerically the NLSE and checked the robustness of two and three-solitons molecules during their evolution. A good agreement is found between the variational calculation and the numerical simulation. Finally, we believe that our findings are appealing for information processing and telecommunication engineering.

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