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Numerically Induced Chaos in the Nonlinear Schrödinger Equation

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The cubic nonlinear Schrödinger equation and some of its discretizations, one of which is integrable, are studied. Apart from the integrable version the discretizations produce chaotic solutions for intermediate levels of mesh (mode) refinement. Chaos disappears when the discretization is fine enough and convergence to a quasiperiodic solution is obtained. Details are given for finite-difference calculations, although similar results are also obtained by Fourier spectral methods. Results regarding a forced nonlinear Schrödinger equation are briefly described.

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The cubic nonlinear Schrödinger (NLS) equation,

$$iu_t + u_{xx} + Q|u|^2u = 0\,, \tag{1}$$

where Q=const, $i^2 = -1$, plays a ubiquitous role in physics. It arises as an asymptotic limit of a slowly varying dispersive wave envelope in a nonlinear medium and as such has significant applications; e.g., nonlinear optics, water waves, plasma physics, etc. Moreover, it has the distinction of being completely integrable via the inverse scattering transform (IST). As such we are ensured that the NLS equation does not possess chaotic behavior for the standard initial-value problem (see Ref. 1 for a review of IST and a discussion of physical applications). Recently there has also been significant interest in particular forced versions of the NLS equation and approximate solutions via low-mode truncations.[2] There are numerous popular discretizations of the NLS equation which provide a vehicle for numerical solutions. Some of these discretizations are physically important in their own right, with applications to nonlinear dimers, self-trapping phenomena, biological systems, etc.[3–5]

The NLS equation and some of its discretizations are excellent models to study the phenomenon of numerically induced chaos. Some advantages are the following: The equation is relatively simple, has known exact solutions (see Refs. 1 and 6), and the discretizations are straightforward. The discretizations we shall consider here are of finite-difference type, although at the end we remark upon another discretization—via Fourier spectral decompositions. We will consider the schemes (assuming periodic boundary conditions, given by $u_{j+N} = u_j$ in the finite-difference case),

$$iu_j + (u_{j+1} + u_{j-1} - 2u_j)/h^2 + Q|u_j|^2 u_j^{(k)} = 0\,, \quad k = 1,2, \tag{2}$$

where (a) $u_j^{(1)} = u_j$ and (b) $u_j^{(2)} = (u_{j+1} + u_{j-1})/2$. Both schemes are of second-order accuracy and Hamiltonian. In case (2a) there are two constants of the motion, the L^2 norm, $I = \sum_{j=0}^{N-1} |u_j|^2$, and the Hamiltonian

$$H = -i \sum_{j=0}^{N-1} \left(|u_{j+1} - u_j|^2/h^2 - \tfrac{1}{2} Q |u_j|^4 \right). \tag{3}$$

Hence, when $N = 2$ the system is integrable. In fact, this system has been used as a model for a nonlinear dimer.[3] The Poisson brackets are the standard ones.

The Hamiltonian structure of scheme (2b) is given (for $h = 1$) by the Hamiltonian[7]

$$H = -i \sum_{j=0}^{N-1} [u_j^*(u_{j-1} + u_{j+1}) = 4Q^{-1} \ln(1 + \tfrac{1}{2} Q u_j u_j^*)]\,, \tag{4}$$

together with the nonstandard Poisson brackets $\{q_m, p_n\} = (1 + \frac{1}{2} Q q_n p_n)\delta_{m,n}$ and $\{q_m, q_n\} = 0 = \{p_m, p_n\}$. This system has been demonstrated to be solvable by IST

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Numerical Chaos, Roundoff Errors, and Homoclinic Manifolds

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The focusing nonlinear Schrödinger equation is numerically integrated over moderate to long time intervals. In certain parameter regimes small errors on the order of roundoff grow rapidly and saturate at values comparable to the main wave. Although the constants of motion are nearly preserved, a serious phase instability (chaos) develops in the numerical solutions. The instability is found to be associated with homoclinic structures and the underlying mechanisms apply equally well to many Hamiltonian wave systems.

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In this Letter we discuss extensive moderate to long time numerical experiments which we have carried out on the focusing nonlinear Schrödinger (NLS) equation with periodic boundary conditions. The NLS equation is a well known Hamiltonian nonlinear wave system which arises in many areas of physics, and is special among such problems since a large class of solutions can be computed via the inverse scattering transform (IST) (e.g., [1]); the NLS equation is said to be "integrable." There are two cases of physical interest—the focusing and defocusing NLS. In the focusing case, when periodic boundary conditions are imposed, the NLS equation has complicated homoclinic structures which under perturbations can produce chaotic dynamics (e.g., [2]). The periodic NLS serves as a useful model describing unstable wave phenomena (e.g., instability in deep water waves) and has been the subject of numerical simulations and laboratory experiments (e.g., [3]).

In our investigations, we employ two numerical schemes which have been used extensively and effectively by researchers studying the NLS equation: (a) the integrable discrete NLS (IDNLS) equation (e.g., [2,4]) and (b) the Fourier split-step (FSS) algorithm (e.g., [5]). The IDNLS equation is an integrable differential-difference equation [4] and is implemented using a high order time discretization. The FSS algorithm, although not integrable, preserves the underlying symplectic structure of the NLS equation and, as such, is in the class of symplectic integrators which have been used as a means of tracking the long time behavior of Hamiltonian systems (e.g., [6] and references therein). We use two numerical schemes to demonstrate that the results obtained are due to the extreme sensitivity of the periodic focusing NLS equation (in the parameter regime described below) and not the particular details of the numerical schemes employed. To be brief we mainly discuss the calculations of IDNLS. The FSS algorithm yields analogous results.

In earlier work we have shown that initial data which are nearby low dimensional "homoclinic manifolds" trigger numerically induced joint spatial and temporal chaos in nonintegrable numerical schemes at intermediate values of the mesh size [2]. This chaos disappears as the mesh is refined. In this Letter we concentrate on a more troubling aspect of numerically induced chaos. We show that temporal instabilities and chaos can be easily excited by very small perturbations—on the order of roundoff. Although our discussion centers on the NLS equation, we have observed analogous behavior in other problems such as the sine-Gordon and modified Korteweg–de Vries (KdV) equations. We believe that similar results will be found in many other Hamiltonian systems. The NLS equation is an excellent paradigm system to study since we have a great deal of analytical knowledge about this equation, and it is reasonably straightforward to compute.

We begin by summarizing our main observations.

(1) Tiny numerical errors (i.e., 10^{-16}) grow rapidly, eventually saturate, but significantly alter the solution after moderate times. For example, spatially even initial values must evolve in an even manner. However, without

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Wave chaos in the nonequilibrium dynamics of the Gross-Pitaevskii equation

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The Gross-Pitaevskii equation (GPE) plays an important role in the description of Bose-Einstein condensates (BECs) at the mean-field level. The GPE belongs to the class of nonlinear Schrödinger equations which are known to feature dynamical instability and collapse for attractive nonlinear interactions. We show that the GPE with repulsive nonlinear interactions typical for BECs features chaotic wave dynamics. We find positive Lyapunov exponents for BECs expanding in periodic and aperiodic smooth external potentials, as well as disorder potentials. Our analysis demonstrates that wave chaos characterized by the exponential divergence of nearby initial wave functions is to be distinguished from the notion of nonintegrability of nonlinear wave equations. We discuss the implications of these observations for the limits of applicability of the GPE, the problem of Anderson localization, and the properties of the underlying many-body dynamics.

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I. INTRODUCTION

Following the experimental realization of Bose-Einstein condensates (BECs) in dilute ultracold gases, the Gross-Pitaevskii equation (GPE), has taken center stage to describe the equilibrium as well as nonequilibrium dynamics of the condensate at the mean-field level [1]. The replacement of the many-body wave function by the effective single-particle condensate wave function has proven to be a remarkably successful approximation for predicting a large variety of physical observables [2]. Among the observables are both ground-state properties and elementary excitations in inhomogeneous background potentials [2–9]. The GPE belongs to the class of nonlinear Schrödinger equations (NLSEs) which have a broad range of applications ranging from nonlinear optics to plasma physics and Bose-Einstein condensation [10]. Effects beyond the GPE have been observed in BECs, most notably in optical lattices with deep wells and small occupation numbers per site. In this regime, explicit many-body descriptions such as the Bose-Hubbard model are more suitable [11,12]. The nonequilibrium dynamics of BECs, specifically their expansion in disordered potentials, has recently received a lot of attention (see, e.g., Refs. [3–9,13–21] and references therein). One focus is on the observation of Anderson localization of a quantum gas. For weak disorder potentials $\langle V\rangle \ll \mu$, where $\langle V\rangle$ is the variance of the potential and μ is the chemical potential of the BEC, the GPE was assumed to be valid during the nonequilibrium expansion starting from the BEC released from the trap to the dilute localized state for which the linear one-particle Schrödinger limit is reached [15,17]. The consequences of the presence of the nonlinearity for the nonequilibrium dynamics in a disordered potential described by the GPE deserves a careful analysis. The NLSE with attractive interactions is known to feature dynamical instabilities leading to collapse of the wave packet [2]. Closely related, the GPE with repulsive pair interaction in a strictly periodic potential features near the Brillouin zone boundary a dynamical (modulation) instability since the effective negative-mass dispersion translates into an effective attractive pair interaction (see, e.g., Refs. [22–26] and references therein). Discretized models resembling the Fermi-Pasta-Ulam-Tsingou[1] system of nonlinearly coupled oscillators have been found to feature stochastic dynamics and relaxation with an increasing entropy [29–31].

We show in the following that the GPE for realistic parameters for the expansion of BECs in the quasi-one-dimensional (quasi-1D) regime displays true wave chaos as measured by a positive Lyapunov exponent in Hilbert space. By careful checks of the accuracy of the propagation including the method of time-reversed propagation, this “physical” chaos can be distinguished from the numerical chaos previously observed for the NLSE [29,32]. We furthermore show that chaos goes beyond the nonintegrability of nonlinear wave equations. The physical consequences of deterministic chaos in the GPE for smooth periodic and aperiodic potentials as well as disorder potentials will be discussed. We argue that wave chaos in the GPE is a signature for the breakdown of mean-field theory and delimits the border of its applicability. The latter does not preclude that certain ensemble expectation values of a BEC can be approximately accounted for by a GPE. We conjecture that the chaotic fluctuations are a signature of excitations and depletion of the condensate. Although our physical interpretations focus on BECs, our findings are relevant for other areas of application of the NLSE as well [33].

The paper is organized as follows. In Sec. II we briefly describe the model for the expansion of a quasi-1D BEC within the GPE. Numerical methods for the propagation of the condensate wave functions are reviewed in Sec. III.

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[1]The model is in literature known under the name Fermi-Pasta-Ulam [27]. We follow here the suggestion by T. Dauxois [28] to recognize the important contribution of M. Tsingou to this pioneering computational study.

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Exponential wave-packet spreading via self-interaction time modulation

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The time-periodic modulation of the self-interaction of a Bose–Einstein condensate or a nonlinear optics system has been recognized as an exciting tool to explore interesting physics that was previously unavailable. This tool is exploited here to examine the exotic dynamics of a nonlinear system described by the Gross–Pitaevskii equation. We observe three remarkable and closely related dynamical phenomena, exponentially localized profile of wave functions in momentum space with localization length exponentially increasing in time, exponential wave-packet spreading, and exponential sensitivity to initial conditions. A hybrid quantum-classical theory is developed to partly explain these findings. Time-periodic self-interaction modulation is seen to be a robust method to achieve superfast spreading and induce genuine chaos even in the absence of any external potential.

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I. INTRODUCTION

Physics induced by the self-interaction of a Bose–Einstein condensate (BEC) or in nonlinear optics has been a fruitful subject. For example, self-interaction on the mean-field level of a BEC often leads to a subdiffusion of cold-atom wave packets, where the second moment of position (or energy) grows as t^{α}, with $0 < \alpha < 1$ [1–10]. Even more remarkable, experimental advances in Feshbach resonance [11–14] or waveguide experiments [15,16] have made it possible to actively tune the self-interaction and then explore new phenomena due to time-modulated self-interaction. In particular, time-periodic modulation of the self-interaction of BECs has been recognized as an exciting tool to engineer the Floquet spectrum [17], control many-body tunneling [18], synthesize novel gauge fields [19], etc. Indeed, the so-called many-body coherent destruction of tunneling [18] has been experimentally realized [20] based on fast time-periodic modulation of the self-interaction strength of cold atoms. In nonlinear optics, the spatial modulation of the Kerr nonlinearity (which can be used to simulate time modulation of nonlinearity) was realized by tuning the refractive index of waveguides with the femtosecond laser writing technique [16].

Here we exploit time-periodic modulation of the self-interaction of an optics system or a BEC on the mean-field level to expose three related dynamical phenomena. The results are of general interest to both theoretical studies and cold-atom-based as well as nonlinear optics experiments. In particular, (i) analogous to the seminal dynamical localization physics [21] in cold-atom realizations of kicked-rotor systems [22], the main localization profile of the time-evolving wave functions in momentum space is found to be exponential; (ii) exponential wave-packet spreading is found to be typical, and its coexistence with exponential wave-function profile is explained in terms of an exponential increase of the localization length in time; (iii) the time evolution is found to be genuinely chaotic because it displays true exponential sensitivity to initial conditions, with the computationally found (finite-time) Lyapunov exponent the same as the rate characterizing the wave-packet spreading for the same timescale. We further use a hybrid quantum-classical theory to shed light on our findings. Our detailed results and theoretical analysis advanced, both quantitatively and qualitatively, a previous work [23] also studying periodic self-interaction modulation.

The exponential wave-packet spreading may offer an alternative route towards superfast heating of particles [24]. Heating up atoms rapidly can suppress the loss of particles from a trap during the heating process. A system of particles after superfast heating, once placed in contact with a cooler system, can be useful for studies of nonequilibrium statistical mechanics. Because the exponential wave-packet spreading is achieved by sole self-interaction modulation in time, it does not need the type of the near-resonance condition advocated in Ref. [25]) and is hence a more robust method than before. Finally, although the dynamics of a system described by the Gross–Pitaevskii equation should be able to exhibit true chaos considering its nonlinear time evolution, this work gives a fascinating example displaying exponential sensitivity without an external potential.

II. MODEL AND RESULTS

Consider a propagating wave under a periodic boundary condition, with its spatial coordinate given by $-\pi \leqslant \theta \leqslant \pi$. Other than the self-interaction that is periodically modulated,

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This isn't from a specialty journal (it's on arXiv), but it's a comprehensive book on BECs and the GPE, *A Primer on Quantum Fluids* by Barenghi and Parker (2016):

Chapter 1

Introduction

Abstract Quantum fluids have emerged from scientific efforts to cool matter to colder and colder temperatures, representing staging posts towards absolute zero (Figure 1.1). They have contributed to our understanding of the quantum world, and still captivate and intrigue scientists with their bizarre properties. Here we summarize the background of the two main quantum fluids to date, superfluid helium and atomic Bose-Einstein condensates.

1.1 Towards absolute zero

The nature of cold has intrigued humankind. Its explanation as a primordial substance, *primum frigidum*, prevailed from the ancient Greeks until Robert Boyle pioneered the scientific study of the cold in the mid 1600s. Decrying the "almost totally neglect" of the nature of cold, he set about hundreds of

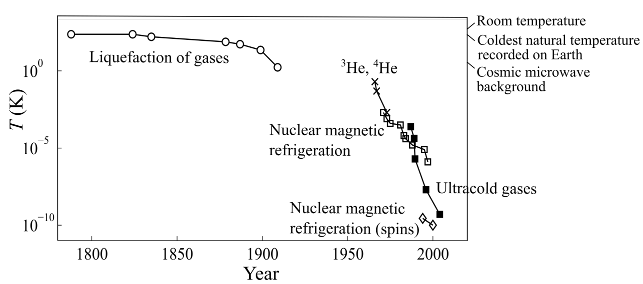

Fig. 1.1 Timeline of the coldest engineered temperatures, along with some reference temperatures.

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experiments which systematically disproved the ancient myths and seeded our modern understanding. While working on an air-based thermometer in 1703, French physicist Guillaume Amontons observed that air pressure was proportional to temperature; extrapolating towards zero pressure led him to predict an "absolute zero" of approximately -240 °C in today's units, not far from the modern value of -273.15 °C (or 0 K). The implication was profound: the realm of the cold was much vaster than anyone had dared believe. An entertaining account of low temperature exploration is given by Ref. [1].

The liquefaction of the natural gases became the staging posts as low temperature physicists, with increasingly complex apparatuses, raced to explore the undiscovered territories of the "map of frigor". Chlorine was liquefied at 239 K in 1823, and oxygen and nitrogen at $T = 90$ K and 77 K, respectively, in 1877. In 1898 the English physicist James Dewar liquefied what was believed to be the only remaining elementary gas, hydrogen, at 23 K, helped by his invention of the vacuum flask. Concurrently, however, chemists discovered helium on Earth. Although helium is the second most common element in the Universe and known to exist in the Sun, its presence on Earth is tiny. With helium's even lower boiling point, a new race was on. A dramatic series of lab explosions and a lack of helium supplies meant that Dewar's main competitor, Heike Kamerlingh Onnes, pipped him to the post, liquifying helium at 4 K in 1908. This momentous achievement led to Onnes being awarded the 1913 Nobel Prize in Physics.

1.1.1 Discovery of superconductivity and superfluidity

These advances enabled scientists to probe the fundamental behaviour of materials at the depths of cold. Electricity was widely expected to grind to a halt in this limit. Using liquid helium to cool mercury, Onnes instead observed its resistance to simply vanish below 4 K. *Superconductivity*, the flow of electrical current without resistance, has since been observed in many materials, at up to 130 K, and has found applications in medical MRI scanners, particle accelerators and levitating "maglev" trains.

Onnes and his co-workers also observed unusual behaviour in liquid helium itself. At around 2.2K its heat capacity undergoes a discontinuous change, termed the "lambda" transition due to the shape of the curve. Since such behaviour is characteristic of a phase change, the idea developed that liquid helium existed in two phases: helium I for $T > T_\lambda$ and helium II for $T < T_\lambda$, where T_λ is the critical temperature. Later experiments revealed helium II to have unusual properties, such as it remaining a liquid even as absolute zero is approached, the ability to move through extremely tiny pores and the reluctance to boil. These two liquid phases, and the fact that helium remains liquid down to $T \to 0$ (at atmospheric pressure), mean that the phase diagram of helium (Figure 1.2) is very different to a conventional liquid (inset).

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Weakly Nonergodic Dynamics in the Gross-Pitaevskii Lattice

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The microcanonical Gross-Pitaevskii (also known as the semiclassical Bose-Hubbard) lattice model dynamics is characterized by a pair of energy and norm densities. The grand canonical Gibbs distribution fails to describe a part of the density space, due to the boundedness of its kinetic energy spectrum. We define Poincaré equilibrium manifolds and compute the statistics of microcanonical excursion times off them. The tails of the distribution functions quantify the proximity of the many-body dynamics to a weakly nonergodic phase, which occurs when the average excursion time is infinite. We find that a crossover to weakly nonergodic dynamics takes place *inside* the non-Gibbs phase, being *unnoticed* by the largest Lyapunov exponent. In the ergodic part of the non-Gibbs phase, the Gibbs distribution should be replaced by an unknown modified one. We relate our findings to the corresponding integrable limit, close to which the actions are interacting through a short range coupling network.

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Equipartition and thermalization are cornerstone concepts of understanding stability and predictability of complex matter dynamics. Proximity to integrable limits may have a strong impact on the needed time scales, or even on equipartition itself. Let us consider a dynamical system which is characterized by a countable set of preserved actions at the very integrable limit, as, e.g., for harmonic lattice vibrations in crystals. Close to the limit, nonintegrable couplings between the actions induce a nontrivial dynamics of the latter. The nonintegrable couplings define a certain connectivity network on the action lattice.

The nonlinear coupling network of the actions can be *long ranged*. That is precisely the case with translationally invariant weakly nonlinear lattice wave equations, or phonon dynamics in crystals, or, e.g., the celebrated Fermi-Pasta-Ulam (FPU) chain [1,2]. Then the linear integrable limit yields actions which are related to standing or plane waves (harmonic phonons) that traverse the entire system. Weak local nonlinearities therefore induce a coupling network which is long ranged [2]. At whatever small, but finite, energy densities in an equipartitioned state, all plane waves and thus actions will be coupled regardless of their characteristics (e.g., the eigenfrequency). Selection rules due to momentum conservation do not alter the above argument. Nature nicely confirms that, since phonon dynamics in crystals appears to be equipartitioned down to the smallest temperatures. At the same time, approaching zero densities will lead to a diminishing of the largest Lyapunov exponent, and thus equipartition times are expected to smoothly diverge in the very limit.

The focus of this work is the case of a Gross-Pitaevskii (GP), also known as Bose-Hubbard (BH), lattice with local nonlinear many-body interactions, and short range hoppings. In the limit of *large* densities the nonlinear interactions dominate over the hoppings, the actions turn local in real space, and the system disintegrates into an uncoupled set of strongly anharmonic oscillators in real space. Close to the limit the short range hoppings induce a nonintegrable *short range* coupling network between the actions. Anomalous and potentially nonergodic large density dynamics was reported for the GP lattice [3–6], including nonequilibrium transport properties [7,8] and self localization [9–11]. Indications for nonergodic dynamics were also observed for similar model classes [12,13].

Strict nonergodic dynamics implies a separation of the phase space into disjoint parts under the action of Hamiltonian dynamics, which could imply the presence of additional symmetries. Such symmetries are unlikely to be restored upon the smooth change of control parameters. An alternative scenario is observed in glassy dynamics, as, e.g., shown by Bouchaud via the appearance of consecutive metastable states, whose lifetimes are distributed according to power-law distributions [14]. If the average lifetime of the metastable states turns infinite, a trajectory might still visit almost all the phase space; however, strictly an infinitely long time is required to observe that when computing averages. Such dynamics, while formally being ergodic, turns *nonergodic* for any finite averaging time. Similar behavior has been discussed by Bel, Rebenshtok, and Barkai in a set of papers dedicated to continuous-time random walks [15–17]. Therein, the phenomenon goes under the name of weak ergodicity breaking, or weak nonergodicity. Lutz further formalized the connection between power-law distribution and weak nonergodicity in the context of optical lattices [18].

The goal of this work is to show the existence of a weak nonergodic phase of the GP lattice dynamics and to

2. The Gross-Pitaevskii equation (GPE) is a nonlinear Schrödinger equation that describes Bose-Einstein condensates (BECs). The equation features a nonlinear addition to the Schrodinger equation approximating the particle interaction as a mean-field Hartree-Fock term. It is interesting that quantum mechanics described by the Schrödinger equation is linear and linearity does not bring chaos—however, classical mechanics routinely shows chaos. Here, chaos is calculated by Lyapunov exponents, the exponential divergence in distances in Hilbert space.

   Here, we characterize chaos within the GPE in one-dimension with Lyapunov exponents. This will be accomplished by simulating the GPE using a finite-differences technique with an adaptive solver. The many-particle wavefunctions will be initialized with turbulence by imparting random phase noise and allowing the function to evolve before perturbing. We will show that chaos is introduced linearly as a function of the interaction term g for positive coupling-term coefficients.

3. Attached.