Modulational instability of a wave scattered by a nonlinear center

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We consider scattering of a quantum particle by a potential which includes a δ function whose amplitude is nonlinear in the wave function. Solution of the scattering problem in this model is nonunique in a certain interval of amplitudes of the incident wave. We demonstrate that the nonlinearity gives rise to an oscillatory instability of the scattering solutions, which is a localized version of the well-known modulational instability of the nonlinear Schrödinger equation. We also consider a nonlinear regime slightly above the instability threshold. The results obtained can be applied to the problem of single-particle tunneling through an ultrashort junction in the presence of multiparticle interaction. Our prediction is that the instability gives rise to an ac component in the transmitted current.

I. INTRODUCTION

A theoretical and experimental study of single-electron tunneling has become a rapidly developing branch of contemporary solid-state physics and physical electronics (see, e.g., the recent review[1]). An important issue is the influence of the many-particle interaction on single-particle tunneling. It was proposed in Ref. 2 that in the simplest approximation of the Hartree type the interaction can be taken into account by adding a phenomenological cubic term to the Schrödinger equation governing the tunneling. Note that a similar effective nonlinear Schrödinger equation (NSE) was employed to describe the dynamics of collective intramolecular excitations (the so-called Davydov solitons) in long polymer chains.[3] In Ref. 2, a NSE with a nonlocal nonlinear term was put forward, and numerical simulations have demonstrated that the nonlinearity gives rise to temporal oscillations. (The first possibility of oscillations in systems of this type was discussed in Ref. 4.) The objective of the present work is to consider this effect analytically in terms of the simplest NSE model,

$$i\psi_t+\psi_{xx}=U(x)\psi+(A+B|\psi|^2)\psi\delta(x)\ . \tag{1}$$

One may regard Eq. (1) as the dimenionless Schrödinger equation governing the single-electron tunneling in an ultrashort junction (heterostructure[2]) represented by the linear term proportional to $\delta(x)$; the many-electron interaction is accounted for by the nonlinear term of the Hartree type. It is assumed that tunneling across the ultrashort junction takes place on the background of some smooth potential $U(x)$. Apart from the tunneling in ultrashort junctions, there are physically meaningful problems of purely classical origin which can also be reduced to the model Eq. (1). One may consider propagation of a linear wave in an inhomogeneous dispersive medium[5] with an inserted strongly nonlinear element. The inhomogeneity gives rise to the potential $U(x)$, while the local nonlinear element is described by the terms proportional to the δ function. Particular examples can be found in dynamical solid-state models,[6] optical wave guides, plasmas, etc.

A fundamental property of the usual NSE is the modulational instability[7] (MI) of its solutions in the case corresponding to $B<0$ (the NSE "with attraction"). It is natural to expect that the localized nonlinearity in Eq. (1) may give rise to a local version of the MI. The objective of the present work is to investigate this effect and its physical consequences. To do this, in Sec. II we first solve the scattering problem for the simplest version of Eq. (1) with $U=0$,

$$i\psi_t+\psi_{xx}=(A+B|\psi|^2)\psi\delta(x)\ . \tag{2}$$

We concentrate on the case $A>0$, $B<0$, when MI is possible. It is implied that the local inhomogeneity repels the particles ($A>0$), while the nonlinear interaction is attractive ($B<0$). This case has nothing to do with the electron tunneling problem, as electrons repel each other, but it can be related to another interesting problem, viz. quantum diffusion of atoms at low temperatures. The latter problem plays an important role in the theory of quantum crystals,[8] where the interaction between the atoms is attractive. As in the case of electron tunneling, we assume that the atoms tunnel across some ultrashort junction in an effectively one-dimensional system.

Of course, direct applicability of the models considered in the present work to the real many-particle tunneling of atoms (in the case $B<0$), as well as to the many-electron tunneling in the case $B>0$ (see below), may seem disputable. However, the common experience gained from analyses of the simplest nonlinear dynamical models demonstrates that they may be quite useful as paradigms which grasp basic qualitative features of the phenomena to be modeled. In particular, a Hartree-type model similar to those analyzed in this work has been very recently set forward in Ref. 9 to model the many-electron quantum dynamics of a heterostructure containing a narrow potential well sandwiched between two narrow potential humps. Numerical simulations of that model reported in Ref. 9 reveal quantum-dynamical chaos which has no classical counterpart. It has been stressed in Ref. 9 that, although the model was introduced phenomenologically, it might be regarded as a simplified version of a more complicated model that could be derived in terms of the screened Coulomb potential.

In Sec. II, we demonstrate that the nonlinearity gives rise to a tristability of solutions of the scattering problem in the model based on Eq. (2) in a certain region of amplitudes of the incident wave. Next, in Sec. III, we consider the stability of the solutions found in Sec. II. We demonstrate that (and this is the central point of the work) localized MI does occur. Unlike MI in the usual NSE, in our case the instability is oscillatory, i.e., it produces an unstable mode oscillating at a certain eigenfrequency that does not depend on the parameter B, i.e., in terms of the underlying physical system, on details of the many-particle interaction modeled by the nonlinear term. Another important difference from the usual MI is that ours has a threshold: it sets in when the amplitude of the scattered wave exceeds a certain threshold (critical) value. Physically, this means that the density of particles in the incident wave must be sufficiently large to excite the MI. The threshold does not depend on the frequency.

For the same model (2), in Sec. IV we consider a weakly overcritical regime when the control parameter lies slightly above its threshold value. We demonstrate that in this regime the wave function ψ contains, as usual, incident, transmitted, and reflected waves, all with the frequency of the incident wave, plus additional transmitted and reflected components with another frequency produced by the instability. Thus, the transmitted current consists of two parts: a large constant one, and a small variable part oscillating at the difference of the two frequencies. The oscillations of the transmitted current is the most important prediction of the present work. We expect that it should be observable in the ultrashort junctions, heterostructures, and in similar systems.

In Sec. V we consider the general model (1) with $U(x)$ in the form of a broad potential barrier. This time, we are interested in the case $A<0$, when a narrow well exists on the background of the broad barrier. The local well gives rise to a discrete quasilevel, and the scattering of the incident wave is resonant when its frequency (the single-particle energy, in terms of the tunneling problem) is close to the quasilevel. The localized MI is apt to occur in this case, and we demonstrate that it exists at any sign of B, unlike the model (2). The results obtained in Sec. V for $B>0$, i.e., for the repelling particles, can be directly applied to the above-mentioned electron tunneling problem which was the motivation for the present work.

II. THE SCATTERING PROBLEM

We start the analysis with the model based on Eq. (2), in which $A>0$ and $B<0$. A scattering solution to this equation is looked for in the form

$$\psi_0(x)=ae^{i\sqrt{\omega}x-i\omega t}+be^{-i\sqrt{\omega}x-i\omega t},\quad x<0 \tag{3a}$$

$$\psi_0(x)=(a+b)e^{i\sqrt{\omega}x-i\omega t},\quad x>0 \tag{3b}$$

where $\omega>0$ is a given frequency. Evidently, the chosen form of the solution satisfies the continuity of the wave function at $x=0$. Integrating Eq. (1) over a small vicinity of $x=0$ yields the following boundary condition (BC) for $\psi(x)$:

$$\psi_x(x=+0)-\psi_x(x=-0)=(A+B|\psi|^2)\psi|_{x=0}\ . \tag{4}$$

The insertion of Eqs. (3) into Eq. (4) yields an equation relating the amplitudes a and b of the incident and reflected waves. This equation can be conveniently represented in the following form. Introduce the parameter μ according to the relation

$$a+b\equiv a/(1+i\mu)\ . \tag{5}$$

Then, Eq. (4) admits real roots μ, which are determined by the equation

$$\mu(1+\mu^2)=(A/2\sqrt{\omega})(1+\mu^2)+(B/2\sqrt{\omega})|a|^2\ . \tag{6}$$

A straightforward analysis demonstrates that the cubic Eq. (6) has three real roots if $AB<0$,

$$A^2>12\omega\ , \tag{7}$$

and $|a|^2$ lies in the interval

$$(4\sqrt{\omega}/27|B|)(A^2/4\omega+3)(A/2\sqrt{\omega}-\sqrt{A^2/4\omega-3})<|a|^2<(4\sqrt{\omega}/27|B|)(A^2/4\omega+3)(A/2\sqrt{\omega}+\sqrt{A^2/4\omega-3})\ . \tag{8}$$

In what follows, the actual control parameter for the stability analysis will be not a, but rather the amplitude $c\equiv a+b$ of the wave function at $x=0$ [see Eq. (3)]. In terms of c, Eqs. (6) and (8) take a simpler form,

$$\mu=A/2\sqrt{\omega}+(B/2\sqrt{\omega})|c|^2\ , \tag{6$'$}$$

$$\tfrac{2}{3}A-\tfrac{1}{3}\sqrt{A^2-12\omega}<|Bc^2|<\tfrac{2}{3}A+\tfrac{1}{3}\sqrt{A^2-12\omega}\ . \tag{8$'$}$$

Further analysis of Eq. (6) yields the bifurcation diagram of the scattering solutions shown in Fig. 1. The diagram takes into account the fact that, according to Eq. (8), the multiplicity of the solution occurs in the finite interval of values of $|a|^2$. It can also be demonstrated that there are two intersections between different branches of the solution which are shown in Fig. 1. Finally, one can identify the branches which are surely unstable and those which may be stable (respectively, dashed and solid lines in Fig. 1) by using the following well-known elementary theorems of the bifurcation theory:[10] (i) when a pair of branches appears "from nothing," one of them must be stable and the other one unstable; (ii) an intersection is

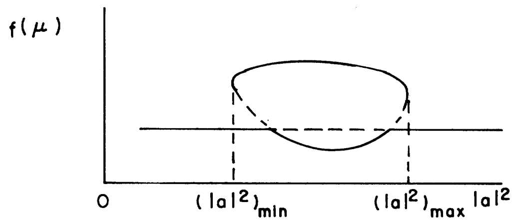

FIG. 1. The schematic bifurcation diagram of the scattering solution. The values $(|a|^2)_{\min}$ and $(|a|^2)_{\max}$ are given by the expressions on the left- and right-hand sides of Eq. (8). $f(\mu)$ is some function of the parameter μ [Eq. (5)] whose particular form is not important.

possible only between stable and unstable branches, and it gives rise to the stability exchange.

III. THE MODULATIONAL INSTABILITY

The solutions shown as stable in Fig. 1 may be actually unstable against modulational perturbations. To investigate the modulational stability, we take the perturbed solution

$$\psi(x,t)=\psi_0(x,t)+\psi_1(x,t) ,$$

where ψ_0 is the stationary solution given by Eqs. (5) and (6) and the infinitesimal perturbation ψ_1 satisfies the linear equation

$$i(\psi_1)_t+(\psi_1)_{xx}=0 \tag{9}$$

off the point $x=0$. At $x=0$, linearization of the full BC (4) yields the BC for Ψ_1,

$$\psi_{1x}(x=+0)-\psi_{1x}(x=-0)=A\psi_1+2B|c|^2\psi_1 + Bc^2\psi_1^* e^{-2i\omega t} , \tag{10}$$

where, as has been defined above, $c\equiv a+b$. Solutions of the linear boundary problem based on Eqs. (9) and (10) are presented in the following form:

$$\psi_1=f_1\exp[(iq-\chi)|x|+(-i\Omega+\Gamma)t] + g_1^*\exp\{(ip-\lambda)|x|+[-(2\omega-\Omega)i+\Gamma]t\} . \tag{11}$$

Evidently, the chosen form of the perturbation ψ_1 satisfies the continuity of ψ at $x=0$ and meets the physical boundary conditions at infinity. There are no new incident waves at $x=\pm\infty$, while new reflected and transmitted waves may appear. The finite value of ψ at $|x|=\infty$ implies that χ and λ in Eq. (11) are non-negative.

Substitution of Eq. (11) into Eq. (9) yields the following relations:

$$\Omega=q^2-\chi^2, \quad 2\omega-\Omega=p^2-\lambda^2 , \tag{12}$$

$$\Gamma=2q\chi=2p\lambda . \tag{13}$$

Next, the BC (10) gives rise to the following equations for the amplitudes f_1 and g_1:

$$2(-iq+\psi)f_1+(A+2Bc^2)f_1+Bc^2g_1=0 , \tag{14a}$$

$$Bc^2f_1+2(ip+\lambda)g_1+(A+2Bc^2)g_1=0 . \tag{14b}$$

(To simplify the notation, it is hereafter assumed that the phase of the complex amplitude a of the incident wave is such that the amplitude c is real.) The resolvability condition for the linear homogeneous system (14) reduces to the following equations:

$$(A+2Bc^2)^2+2(A+2Bc^2)(\chi+\lambda)+4\chi\lambda+4pq=B^2c^4 , \tag{15}$$

$$2(q\lambda-p\chi)+(A+2Bc^2)(q-p)=0 . \tag{16}$$

Equations (12), (13), (15), and (16) constitute a system of equations for the six unknown parameters Ω, p, q, χ, λ, and Γ. Since the underlying equation (1) is a Hamiltonian, the stability of the stationary solutions may be only neutral, i.e., they are stable as long as $\Gamma=0$. From Eq. (13), the stability requires $\chi=\lambda=0$, i.e., there must be no localized eigenmodes. The instability sets in when there appear infinitesimal positive χ and λ. The goal of the further analysis is to find out how this happens. To that end, we assume χ and λ to be nonzero but vanishingly small. Using the relation $p/q=\chi/\lambda$ ensuing from Eq. (13), we exclude p and q from Eq. (16) to arrive at the equation

$$(p-q)[\chi+\lambda+\tfrac{1}{2}(A+2Bc^2)]=0 . \tag{17}$$

As it follows from Eq. (17), there are two possibilities—either $p=q$ or

$$\chi+\lambda=-\tfrac{1}{2}(A+2Bc^2) . \tag{18}$$

In the former case, it immediately follows from Eqs. (12) and (13) that $\chi=\lambda$ and $\Omega=\omega$. The latter relation implies that this mode of the instability gives rise to no new frequency. Then one finds from Eq. (15)

$$\chi=\lambda=-\tfrac{1}{4}(A+2Bc^2) \pm\tfrac{1}{2}(-ABc^2-\tfrac{1}{4}A^2-\tfrac{1}{2}B^2c^4-2\omega)^{1/2} \tag{19}$$

(recall that we assume $A>0$, $B<0$). The instability exists when at least one root (19) is real and positive. It is straightforward to see that this takes place exactly when c^2 belongs to the interval (8′). Thus, this mode of the instability should be closely related to the bifurcations shown in Fig. 1, and a subsequent analysis demonstrates that this instability is exactly that which is responsible for the bifurcations.

A nontrivial instability mode is generated by Eq. (18). According to Eq. (18), positive A yields no instability if $B>0$. This complies with the well-known fact that in the usual NSE "with repulsion" ($B>0$) there is no modulational instability.[2] If $B<0$, the instability sets in when the amplitude attains the critical value given by the expression

$$(|B|c^2)_{\rm cr}=\tfrac{1}{2}A . \tag{20}$$

It is easy to find that, at this point, the wave numbers of the critical disturbance are

$$(p,q)_{\rm cr}=\tfrac{1}{2}[(2\omega+\tfrac{1}{8}A^2)^{1/2}\pm(2\omega-\tfrac{1}{8}A^2)^{1/2}] , \tag{21}$$

and the instability is oscillatory, i.e., it gives rise to the pair of new frequencies

$$(\Omega, 2\omega-\Omega)_{\rm cr}=\omega \pm \sqrt{\omega^2-(A^2/16)^2}\ . \tag{22}$$

Note that the threshold amplitude (20) does not depend on ω, while the critical frequencies (22) do not depend on B.

The present instability exists if

$$A^2 \le 16\omega\ . \tag{23}$$

In the region $A^2<12\omega$, the bifurcations shown in Fig. 1 are absent (the scattering solution is unique), and only the oscillatory instability occurs. In the region $12\omega \le A^2 \le 16\omega$, the scattering solution may be subject to both instabilities; however, one can readily demonstrate that in this case the oscillatory instability always sets in prior to the bifurcation, i.e., at a smaller value of c^2. Finally, the oscillatory instability is absent in the region $A^2>16\omega$ [see Eq. (23)].

IV. THE WEAKLY NONLINEAR ANALYSIS OF OSCILLATORY INSTABILITY

The nonlinear stage of development of the oscillatory instability can be analyzed in the weakly overcritical case, when the amplitude of the underlying stationary wave lies slightly above the critical value (20),

$$0<\delta \equiv |B|c^2-\tfrac{1}{2}A \ll \tfrac{1}{2}A\ . \tag{24}$$

We assume that $f_1, g_1 \sim \sqrt{\delta}$. The amplitudes can be found if one closes equations of the perturbation theory at the order $\sim \delta^{3/2}$. To do this, one should first proceed to the order $\sim\delta$. At this order, it is necessary to add the combinational harmonics to the linear eigenmode (11),

$$\psi_1=f_1 e^{iq_1|x|-i\Omega_1 t}+g_1^* e^{ip|x|-i(2\omega-\Omega_1)t} +f_2 e^{iq_2|x|-i(2\Omega_1-\omega)t}+g_2^* e^{ip_2|x|-i(3\omega-2\Omega_1)t} +h_2 e^{i\sqrt{\omega}|x|-i\omega t}\ , \tag{25}$$

where Ω_1 is assumed to be close to the critical value given by Eq. (22), $q_1 \equiv \sqrt{\Omega_1}$, $p_1 \equiv \sqrt{2\omega-\Omega_1}$, $q_2 \equiv \sqrt{2\Omega_1-\omega}$, $p_2 \equiv \sqrt{3\omega-2\Omega_1}$, and the amplitudes f_2, g_2, and h_2 are assumed to be $\sim\delta$. Inserting $\psi \equiv \psi_0+\psi_1$ into the nonlinear BC (4) and equating coefficients in front of the combinational harmonics, one can express f_2, g_2, and h_2 as quadratic combinations of f_1 and g_1. Next, closing the perturbative expansion for the fundamental harmonics (those with the frequencies Ω_1 and $2\omega-\Omega_1$) at order $\delta^{3/2}$, one arrives at the equations (14) with the nonlinear corrections $\sim\delta^{3/2}$. As the coefficients of Eqs. (14) are complex, the resolvability condition for the corresponding nonlinear equations should give two real equations to determine $|f_1|^2 \sim \delta$ and the frequency shift $\Omega_1-\Omega_{\rm cr} \sim \delta$. Next, the relation between g_1 and f_1 can be derived from Eqs. (14) at the critical point

$$g_1=-(4iq_{\rm cr}/A)f_1\ . \tag{26}$$

In a general case, the eventual expressions are very cumbersome. So, consider the case $A^2 \ll 16\omega$ [cf. Eq. (23)]. Then, $\Omega_1 \simeq 1/2\omega(A^2/16)^2$, $q_1 \simeq A^2/16\sqrt{2\omega}$, $p_1 \simeq \sqrt{2\omega}$, and, finally, in the lowest approximation one obtains

$$|f_1|^2=2\delta/|B|, \Omega_1-\Omega_{\rm cr}=0\ . \tag{27}$$

Thus we conclude that the oscillatory instability gives rise to an ac component in the full current $j \equiv i\psi_x\psi^*$ with the amplitude $\sim\sqrt{\delta}$, oscillating at the beating frequency $\Omega_{\rm cr}-\omega=\sqrt{\omega^2-(A^2/16)^2}+O(\delta)$.

V. THE MODULATIONAL INSTABILITY ON THE BACKGROUND OF A SMOOTH POTENTIAL

Let us consider the model (1), which includes the smooth potential $U(x)$ and a local potential well ($A<0$). In this well, one can get a discrete quasilevel, whose wave function is localized near $x=0$. If its localization length is much smaller than a characteristic scale of the smooth potential $U(x)$, the quasilevel exists at the value of the single-particle energy (frequency)

$$\omega_0=U_0-\tfrac{1}{4}A^2\ , \tag{28}$$

where $U_0=U\ (x=0)$. It is well known that the resonance takes place when the incident wave has a frequency ω close to ω_0: The wave function grows exponentially inside the barrier, reaching a maximum value at $x=0$. As we have seen above, the instability sets in when the amplitude of the wave at $x=0$ attains a certain threshold value. Therefore, in what follows we confine ourselves to the case $\omega=\omega_0$.

We again seek for the eigenmode of the stability problem in the general form (11). The same equations, (12)–(16), remain valid if one replaces ω by $\omega_0-U_0 \equiv -\frac{1}{4}A^2$ [see Eq. (28)]. However, the eigenmode is now localized inside the barrier, so that the stability condition $\Gamma=0$ holds as long as $p=q=0$, while χ and λ are positive [see Eq. (13)]. To find the instability threshold, we again use Eq. (18), which at the threshold (with infinitesimal p and q) takes the form

$$\sqrt{U_0-\Omega}+(\tfrac{1}{2}A^2-U_0+\Omega)^{1/2}=-\tfrac{1}{2}(2Bc^2+A)\ . \tag{29}$$

Equation (29) should be combined with Eq. (15), which reads at the threshold

$$\sqrt{U_0-\Omega}(\tfrac{1}{2}A^2-U_0+\Omega)^{1/2}=\tfrac{1}{4}B^2c^4\ . \tag{30}$$

Excluding the frequency Ω, one finds from Eqs. (29) and (30) that the instability sets in at

$$(Bc^2+A)^2=\tfrac{3}{2}A^2\ . \tag{31}$$

Recall that in the model (2) the instability exists only at $B<0$. Now the situation is different. By virtue of Eq. (31), at $B<0$ the instability threshold lies at

$$|B|c^2=(\sqrt{3/2}-1)|A| \simeq \tfrac{2}{9}|A|\ ; \tag{32a}$$

at $B>0$ it lies at

$$Bc^2=(\sqrt{3/2}+1)|A| \simeq \tfrac{22}{9}|A|\ . \tag{32b}$$

Analysis of the weakly nonlinear stage can also be developed for the "underbarrier" instability. However, it cannot be presented in a universal form. Indeed, the nonlinear analysis should determine two quantities: The amplitude $|f_1|^2$ of the disturbance and the frequency shift $\Omega_1-\Omega_{cr}$ (see Sec. IV). However, Eqs. (14), written for the localized (exponentially decaying) wave function ψ_1, have purely real coefficients, so one arrives at one equation for $|f_1|^2$ and $\Omega_1-\Omega_{cr}$. To lift this degeneracy, one should take into account the exponentially small components of the wave function under the barrier. In principle, this can be done, but the result depends upon a particular shape of the smooth potential $U(x)$.

VI. CONCLUSION

In this work, we have found the localized modulational instability (MI) generated by the localized nonlinearity in the Schrödinger equation. Unlike the instability in the usual NSE, the localized MI is oscillatory, and it has the threshold. We expect that this instability occurs in a broad class of models. For instance, the numerical simulations reported in Ref. 2 demonstrated essentially nonlinear oscillations in the Schrödinger equation with a nonlocal nonlinear term, governing resonant tunneling of a Gaussian pulse through a double barrier (see also Ref. 9).

Our general conclusion can be formulated as follows. The many-particle interactions in mesoscopic systems (ultrashort junctions, etc.[1]) should give rise to the MI of the wave function, which will manifest itself by the ac component of the transmitted current in the dc-driven systems. We believe that the search for this effect could be a relevant problem. As was said above, one can expect that the variant of our model with attraction between the particles should be a phenomenological model for diffusion of atoms in a quantum crystal, while that with repulsion directly applies to the tunneling of electrons through ultrashort junctions. An experimental realization in other types of heterostructures may be feasible also.[2,9]

To give some idea of the conditions necessary for this effect to be observed, let us note, first of all, that the frequencies (22), at which MI sets in the system with attraction, do not depend on the parameter B, i.e., on details of the many-particle interaction accounted for by the nonlinear term. According to Eq. (20), one should provide for a sufficiently high density of the particles in the incident wave to excite the instability. Simultaneously, Eq. (23) tells us that the frequency ω, i.e., the single-particle energy in the incident wave, must be sufficiently large also. It is also noteworthy that the threshold density of the particles necessary to excite MI [Eq. (20)] does not depend on the single-particle energy. Both Eqs. (20) and (23) imply that, the weaker the short potential barrier characterized by parameter A, the easier it must be to observe the effect.

If one is searching for the effect predicted on the background of the broad potential barrier $U(x)$ (in particular, in the case of the repulsive interparticle interaction), it is necessary, as emphasized in Sec. V, to choose the single-particle energy close to the value of the quasilevel generated by the narrow potential well. Note that in this case the critical frequencies also do not depend on the parameter B [see Eqs. (29)–(32)].

As mentioned in the Introduction, the same effect can also be realized in purely classical dispersive media with an inserted nonlinear element. Deeper into the unstable region, the development of the instability may give rise to dynamical chaos. However, investigation of the deeply unstable region should be done numerically (recently, chaotic dynamics in a model similar to ours were observed in the numerical simulations reported in Ref. 9).

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