

Theory of nonlinear oscillating dipolar excitations in one-dimensional condensates

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We find that for a one-dimensional condensate in the presence of an applied ac field, a significant absorption peak should occur for values of the external frequency just below the pinning frequency ω_F . This power absorption is due to those nonlinear normal modes of the condensate known as "breathers," which are shown to phase lock with the applied field.

I. INTRODUCTION AND DISCUSSION

In a recent Letter¹ Rice, Bishop, Krumhansl, and Trullinger (RBKT) suggested that solitary waves in a one-dimensional condensate, such as Tetrathiafulvalenium-tetracyanoquinodimethanide (TTF-TCNQ), could give a significant contribution to the dc conductivity at low temperatures. These solitary waves, called " ϕ particles," are localized charge-density waves possessing a total charge of $\pm e^*$. If the system dynamics is described by the sine-Gordon equation,²⁻⁴ then these solitary waves are solitons (i. e., they retain their identities through collisions) and are called kinks and antikinks, or 2π pulses. Of course, it is also well recognized that the actual physical potential probably is not an exact sine-Gordon potential, in which case these localized kinklike solutions are only solitary waves, not solitons. However, even if this is the case, there is always another nonlinear mode in systems such as these that for sufficiently small amplitude of oscillations is a true soliton. In addition, we must point out that, although this nonlinear mode does have a small amplitude, it will still be nonlinear due to its long range. We shall return to this point later. When the potential is a sine-Gordon potential, this nonlinear mode is always a soliton (i. e., under collisions it loses no energy or momentum) for any amplitude, small or large, and is called a breather,² or 0π pulse. Unlike the kink, the breather requires no activation energy, and its energy can range continuously from zero to $2Mc_0^2$, where Mc_0^2 is the rest energy of the kink or antikink. Furthermore, although the total charge carried by the breather is zero, it is an oscillating state and corresponds in the RBKT model to an oscillating electric dipole. It is the purpose of this paper to show that breathers can be stimulated by, and can synchronize to, an external ac forcing field with a frequency below the pinning frequency of the medium, and to suggest that at low temperatures they may be responsible for a significant amount of the ac-current-carrying capacity of the condensate. Although the initial part of our discussion

will be in terms of the sine-Gordon model, again we must point out that our theory will be applicable for a very broad range of potentials.

Using the sine-Gordon potential in the RBKT one-dimensional model, the local phase $\phi(x, t)$ is described by

$$\ddot{\phi} - c_0^2 \phi'' + \omega_F^2 \sin\phi = 0, \quad (1)$$

for which the breather solution² is

$$\phi(x, t) = 4 \tan^{-1}(A \cos\omega T) / \cosh(2\eta X), \quad (2)$$

where

$$A = 2\eta c_0 / \omega, \quad (3a)$$

$$\omega^2 = \omega_F^2 - 4\eta^2 c_0^2, \quad (3b)$$

and

$$T = \gamma(t - vx/c_0^2), \quad (4a)$$

$$X = \gamma(x - vt), \quad (4b)$$

$$\gamma = (1 - v^2/c_0^2)^{-1/2}. \quad (4c)$$

Note that the natural frequency of the breather depends on its amplitude and lies *below* ω_F . Also note that the amplitude and width are inversely related, such that this pulse has an absolute area on the order of c_0/ω . For small amplitudes, it has a wide structure, and by referring to Eq. (1), one can easily see how this is happening when $|\phi| \ll 1$. For this pulse, the second term in Eq. (1), the dispersion, is of the order of $\eta^3 c_0^3/\omega$, while the nonlinearity in the $\sin\phi$ term is of the same order. Thus there occurs a balance between the dispersion and nonlinearity.

On the other hand, the phonon solution of Eq. (1) corresponding to the linear dispersive wave of wave number k and frequency ω_{ph} , is

$$\omega_{ph}^2 = \omega_F^2 + c_0^2 k^2, \quad (5)$$

which lies *above* ω_F . In this solution, there is no balance between the dispersion and nonlinearity, and the wave is essentially dispersive in character. What happens here is that the phasing between the dispersion and nonlinearity is the same, so that both terms act to push the wave apart and

to disperse it. Thus for suitably wide disturbances one can expect both of these solutions to be present, with the nonlinearity "splitting" the energy levels. The breather is like a bound state with a frequency [Eq. (3b)] below ω_F , while the nonlinear phonon state has a frequency [Eq. (5)] above ω_F . [There are nonlinear wave-train solutions of Eq. (1) whose frequency is less than ω_F due to nonlinear frequency modulation (or shift), but these are *unstable* and relax to the lower-energy states, which are the breather modes.] Consequently, in any experiment involving frequencies close to ω_F , we would expect contributions from both the phonon and breather modes, the latter (stable modes) being exclusively responsive to frequencies $\omega \approx \omega_F$.

From the phenomenological theory of such systems,^{5,6} the local current and charge densities are given by

$$j(x, t) = n_s e q_0^{-1} \dot{\phi}(x, t), \quad (6a)$$

$$\rho(x, t) = -n_s e q_0^{-1} \phi'(x, t), \quad (6b)$$

where n_s , e , and q_0 are the density of condensed conduction electrons, their charge, and the fundamental periodicity of the undeformed condensate, respectively. If we use the sine-Gordon breather solution, Eq. (2), in Eq. (6b), since the total change in ϕ from $x = -\infty$ to $x = +\infty$ is zero (unlike the kink solution where it is 2π), the total charge $\int_{-\infty}^{\infty} \rho(x, t) dx$ of the breather is zero (for the kink it is a finite constant e^*); however, the dipole moment $p_s(t) = \int_{-\infty}^{\infty} x \rho(x, t) dx$ is not zero. From Eq. (2), it follows that in the rest frame of the breather

$$p_s(t) = (\pi e n_s / 2 q_0 \eta) \sinh^{-1}(A \cos \omega t), \quad (7)$$

which for a low-amplitude breather reduces to $p_s = (\pi e c_0 n_s / q_0 \omega) \cos \omega t$, which is independent of the amplitude and has only one frequency component. But for large amplitudes, this moment will be amplitude dependent and will contain ω and all of its higher odd harmonics.

From the Lagrangian for the sine-Gordon model,¹ one can determine the Hamiltonian, which then gives the rest mass of the breather as being

$$M_b = 2M(1 - \omega^2/\omega_F^2)^{1/2}, \quad (8)$$

where M is the kink or antikink effective mass, which is

$$M = 8n_s m^* \omega_F / (c_0 q_0^2). \quad (9)$$

For $\omega = 0$ the rest mass M_b is the same as that for a kink plus antikink, and as ω approaches ω_F , it goes to zero and therefore would require no activation energy. One can thus formally consider the breather as being a bound state of a kink-antikink pair, and then the oscillating dipole moment may be simply interpreted as the natural plasmalike

oscillation between the positively and negatively charged regions.

At low temperatures, since the activation energy for a breather can be very small, and even almost zero, we can expect the density of breathers to be reasonably large, perhaps even close to the density of phonons. So it is of considerable interest to determine whether or not they can be experimentally observed, and to determine how they could affect the properties of a system. Clearly, since low-amplitude breathers have a natural frequency just below ω_F , we want to look at the properties of these solitons in the presence of an applied ac electric field, where $\omega \lesssim \omega_F$. And, to make the calculations a little more physical, we shall introduce also a phenomenological viscous damping.

II. ANALYSIS

Before calculating the effects of damping and the applied field on these breathers, it is first advisable to reduce a generalization of Eq. (1) to a more generic form, using a small-amplitude approximation, and to discuss carefully some of the more important features of this generic equation. After we do this, we shall consider the damping and applied field as perturbations, and calculate their long-time effects on the breathers to first order. Although there exist well-developed perturbation theories for handling such perturbations,⁷⁻⁹ we shall derive these effects by a much simpler method, by using the first two of the infinity of conservation laws. The advantage of this is that it quickly gives the correct answer and works whenever the continuous spectrum (phonons) does not resonate with either the perturbation or the solitons.

These conditions will be satisfied in this case, because we shall assume explicitly that the frequency of the applied field is less than ω_F . Our calculations show that the breather can "phase lock" onto the applied field, drawing energy out of the field. The conditions for phase locking to occur will be discussed, and then we shall give some numerical estimates of the size of this effect in TTF-TCNQ.

The generalized form of Eq. (1), in the notation of RBKT, is

$$\ddot{\phi} + \Gamma \dot{\phi} - c_0^2 \phi'' + \omega_F^2 \frac{dV}{d\phi} = -2\omega_F \epsilon \cos \omega_0 t, \quad (10)$$

where Γ is the phenomenological viscous damping constant,

$$\epsilon = 2e^* E / \pi M c_0, \quad (11)$$

and the ac electric field has been taken to be $-E \cos \omega_0 t$, with ω_0 as its central frequency. Also, we are now considering a more general case than the sine-Gordon model by allowing $V(\phi)$ to be fair-

ly arbitrary (in the sine-Gordon model $V = 1 - \cos\phi$). In general, for small amplitudes, $V(\phi)$ will have the Taylor-series expansion,

$$V(\phi) = \frac{1}{2}\phi^2 - \frac{1}{24}\alpha^2\phi^4 + \gamma\phi^5 + \dots \quad (12)$$

Cubic terms in the expansion for $V(\phi)$ may be included. In a small amplitude expansion, they will produce second harmonics and a possible dc field, both of which in turn will interact with the fundamental, and the net effect will be to modify the coefficient of the quartic term in $V(\phi)$. We assume only that the (effective) coefficient of ϕ^4 is negative, the "soft" spring case. In the sine-Gordon model $\alpha^2 = 1$, so α^2 will be a measure of the deviation of $V(\phi)$ from the sine-Gordon model. However, we should also emphasize again that our results will be valid for *any* value of $\alpha^2 > 0$, and thus the errors in our small amplitude approximation shall only be in the fifth order [which is absent if $V(\phi)$ is even] or the sixth order.

To reduce Eq. (10) to a more generic form, we note from Eqs. (2) and (3) that for low-amplitude breathers the frequency of the natural oscillation of ϕ is very close to ω_F , and thus we may let

$$\phi(x, t) = \text{Re}[\psi(x, t)e^{-i\omega_F t}]. \quad (13)$$

Inserting Eqs. (12) and (13) into Eq. (10), and (i) assuming that the time variations in ψ are much longer than ω_F^{-1} (exactly the same approximation that is used to derive the nonrelativistic Schrödinger equation from either the Klein-Gordon or the Dirac equation), (ii) assuming that all "fast" time ($\omega_F t$) variations average out, and (iii) retaining only the first two terms in Eq. (12), one obtains

$$i\psi_t = - (c_0^2/2\omega_F)\psi'' - \frac{1}{16}\alpha^2\omega_F\psi^*\psi^2 - \frac{1}{2}i\Gamma\psi + \epsilon e^{i\delta\omega t}. \quad (14)$$

where

$$\delta\omega = \omega_F - \omega_0. \quad (15)$$

For the moment, ignore the last two terms in Eq. (14). Then Eq. (14) is simply the "nonlinear Schrödinger (NLS) equation",¹⁰ which for $\alpha^2 > 0$,¹¹ has soliton solutions of the form

$$\psi(x, t) = (8c_0\eta/\alpha\omega_F) \text{sech}\theta e^{i\sigma}, \quad (16)$$

where

$$\theta = 2\eta(x - x_0 - vt), \quad (17a)$$

$$\sigma = -2\xi x - 2c_0^2\omega_F^{-1}(\xi^2 - \eta^2)t + \sigma_0, \quad (17b)$$

with the velocity given by

$$v = -2c_0^2\xi/\omega_F. \quad (18)$$

Comparison of Eqs. (2) and (16) shows that in the low-amplitude limit, the sine-Gordon breather is equivalent to a NLS soliton, but now Eq. (16) ap-

plies to a much wider class of systems than does the sine-Gordon model.

Now, a careful reader may well ask why should we consider this soliton solution at all, since it is clear that Eq. (14) has exact nonlinear plane-wave solutions with frequencies less than zero [and thus $\phi(x, t)$ has a frequency less than ω_F] in the absence of the forcing term and damping. That is indeed true, but *all* such plane-wave solutions are *modulationally unstable*,⁷ and will, with a growth rate on the order of $\alpha^2\omega_F\psi^*\psi$, decay into these soliton solutions and the "nonlinear phonon" modes. Thus in any general system, such as given by Eqs. (10) and (12), the solitons will be the *stable* configurations, whereas plane waves will be unstable.

Let us now turn our attention to the crux of the problem, which is to determine the long-time first-order effects of the damping and forcing terms on the soliton solutions of Eq. (14). Currently, there are well-developed methods^{8,9} for doing this in the context of the inverse scattering transform. These methods are very general, and are based on the fact that the inverse scattering transform is a canonical transform, transforming the field into the action-angle variables, which are the "scattering data." However, for the one-soliton solution, there is a much more direct method for obtaining the final result, which we shall now illustrate and use. (Nevertheless, sometimes this more direct method can give misleading results, especially if the continuum spectrum can be excited and contribute to the conserved quantities. For an example, see Ref. 9. However in the present case, no such difficulties occur.)

Every system solvable by the inverse scattering transform has an infinity of conserved quantities, the first two of which, for the NLS, are

$$C_1 = \int_{-\infty}^{\infty} \psi^*\psi dx, \quad (19a)$$

and

$$C_2 = i \int_{-\infty}^{\infty} (\psi^*\psi' - \psi'^*\psi) dx. \quad (19b)$$

From the inverse-scattering-transform theory, one can show that each of these conserved quantities is an *additive* function of the corresponding quantities for each soliton, and for each phononlike "mode." In other words, although the NLS is a nonlinear equation, the total momentum, energy, etc., of the system is simply a linear sum of the corresponding quantities for each soliton and each phonon mode. Thus in the absence of any perturbations, there is never any "real" interaction between these modes. Therefore, if we start with only one soliton, no phononlike modes can buildup except through the interaction of the soliton with

the perturbation. However, if $\omega_0 < \omega_F$, the phonon modes will be nonresonant with the forcing term, whereas the solitons will be resonant. So, one can then expect that if C_n is initially pure soliton in character, it then will continue to remain essentially pure soliton in character.

Now, consider the time rate of change of Eqs. (19), which, when the perturbations are present [Eq. (14)], gives

$$\dot{C}_1 = -\Gamma C_1 - \epsilon I_1, \quad (20a)$$

$$\dot{C}_2 = -\Gamma C_2, \quad (20b)$$

which are exact relations, with

$$I_1 = 2\text{Im} \left(e^{-i6\omega t} \int_{-\infty}^{\infty} \psi dx \right). \quad (21)$$

When ψ remains pure soliton in character, as in Eq. (16), then by Eqs. (19),

$$C_1 = 64c_0^2 \eta / (\alpha \omega_F)^2, \quad (22a)$$

$$C_2 = 256c_0^2 \eta \xi / (\alpha \omega_F)^2, \quad (22b)$$

so that by Eq. (20b), $\eta \xi \rightarrow 0$, regardless of the forcing term. This simply says that either the soliton's amplitude or its velocity must vanish due to the viscous damping. Thus, without loss of generality, we may take $\xi = 0$, and also $x_0 = 0$. Then evaluation of Eqs. (21) and (20a) gives

$$\dot{\eta} + \Gamma \eta = (\alpha \pi \epsilon \omega_F / 8c_0) \sin(\delta\omega t - \sigma). \quad (23a)$$

The time rate of change of σ to first order in the perturbation must follow from more-general inverse scattering methods,^{8,9} but since we only need the lowest-order nonzero terms, which for σ is the zeroth-order term, inspection of Eq. (17b) shows this to be simply

$$\dot{\sigma} = 2(c_0^2 / \omega_F) \eta^2. \quad (23b)$$

Equations (23) are easy to interpret. Equation (23a) shows that the damping tries to cause the soliton to decay in amplitude, while the ac electric field can either work with or against the damping, depending on the instantaneous phase difference between the soliton and the forcing term. Meanwhile, and very importantly, the soliton's frequency $\dot{\sigma}$ changes as its amplitude changes, as shown by Eq. (23b). In such a situation, it is possible for the soliton to "phase lock" onto the applied ac electric field by adjusting its frequency, and to draw energy out of the field. For this to occur, $\dot{\sigma} = \delta\omega$, which then gives

$$\sigma = \delta\omega t - \chi_0, \quad (24a)$$

$$\eta = (\frac{1}{2} \delta\omega \omega_F / c_0^2)^{1/2}, \quad (24b)$$

$$\sin \chi_0 = (8\Gamma / \alpha \pi \epsilon) (\frac{1}{2} \delta\omega / \omega_F)^{1/2}, \quad (24c)$$

where χ_0 is the phase-locked phase difference between the soliton and the applied field. Note from

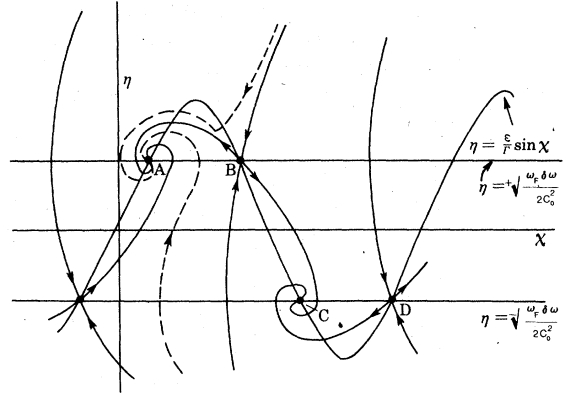


FIG. 1. Phase-plane trajectories for Eqs. (23), with $\chi = \delta\omega t - \sigma$ and $\epsilon = \alpha \pi \epsilon \omega_F / 8c_0$.

Eq. (24c) that this phase locking will not occur unless $\delta\omega$ is sufficiently small, or

$$0 < \delta\omega < \Delta\omega, \quad (25)$$

where the frequency window $\Delta\omega$ is given by

$$\Delta\omega = \frac{1}{32} \alpha^2 \pi^2 (\epsilon / \Gamma)^2 \omega_F. \quad (26)$$

Computer solutions of Eqs. (23) have shown that this phase locking, when it occurs, occurs quite rapidly, and a typical result for the phase plane of η vs χ , where

$$\chi = \delta\omega t - \sigma, \quad (27)$$

is shown in Fig. 1, the singular points (A, C) are stable nodes (and also "spiral points") for Eqs. (23), while the companion singular points (B, D) are unstable saddle points. Two typical trajectories are indicated by the dotted lines. Of course, all points in Fig. 1 for $\eta < 0$ must be discounted, since solitons only correspond to $\eta > 0$. Any orbit which passes into this lower-half η plane presumably corresponds to a soliton decaying down into phonons. Whether or not the soliton would reform out of the phonons so formed if the orbit moves back up into the upper-half η plane is unknown at the moment.

To understand further the behavior of the solution about these singular points, one can easily derive a quasilinear second-order differential equation for χ about these points. From Eqs. (23) and (27), assuming $|\chi| \ll \delta\omega$ so that $\eta \approx c_0^{-1} (\frac{1}{2} \omega_F \delta\omega)^{1/2} (1 - \frac{1}{2} \chi / \delta\omega)$, it then follows that

$$\ddot{\chi} + \Gamma_{\text{eff}} \dot{\chi} + \frac{dU(\chi)}{d\chi} = 0, \quad (28a)$$

where

$$\Gamma_{\text{eff}} = \Gamma [2 - (\Delta\omega / \delta\omega)^{1/2} \sin \chi], \quad (28b)$$

$$U = -2\Gamma \delta\omega [\chi + (\Delta\omega / \delta\omega)^{1/2} \cos \chi]. \quad (28c)$$

Equation (28) corresponds to a damped particle

moving in a potential U . This potential has a periodic part and a linear part, where the latter has a negative slope. The unstable singular point (B) corresponds to the local maxima of Eq. (28c), which are given by

$$\chi_0 = \pi - \sin^{-1}(\delta\omega/\Delta\omega)^{1/2} + 2\pi m, \quad (29)$$

while the stable spiral point (A) corresponds to the local minima of Eq. (28c), given by

$$\chi_0 = \sin^{-1}(\delta\omega/\Delta\omega)^{1/2} + 2\pi m. \quad (30)$$

Power will be absorbed by a NLS soliton in a time-averaged sense only when phase locking occurs. From Eqs. (6), (13), (16), (17), (24), (30), and the definition of the applied electric field following Eq. (11), we have

$$\begin{aligned} \langle P \rangle &= - \left\langle E \int_{-\infty}^{\infty} dx j(x, t) \cos\omega_0 t \right\rangle, \\ &= \frac{1}{2} \pi \alpha^{-1} M c_0^2 \epsilon \sin\chi_0, \\ &= 2\alpha^{-2} \Gamma M c_0^2 (2\delta\omega/\omega_F)^{1/2}, \end{aligned} \quad (31)$$

and where we have assumed $\omega_0 \simeq \omega_F$. Note that the power absorbed is independent of the strength of the applied field, since $\epsilon \sin\chi_0$ is independent of ϵ .

III. CONCLUSIONS

These results have several interesting consequences. If at a fixed frequency less than ω_F the amplitude E of the applied field is slowly increased from zero, $\langle P \rangle$ remains zero until the threshold given by

$$e^* E = 2\Gamma \alpha^{-1} M c_0 (2\delta\omega/\omega_F)^{1/2} \quad (32)$$

is reached. At this point phase locking can occur, and $\langle P \rangle$ will suddenly increase to the nonzero value given by Eq. (31), and will remain at this level, regardless of the subsequent amplitude of E . On the other hand, if E is kept fixed and ω_0 is varied slowly downward through ω_F , then for $\omega_0 > \omega_F$, only the phonon spectrum is excited. However, once ω_0 decreases below ω_F , then $\langle P \rangle$ is given by Eq. (31), which is now frequency dependent but amplitude independent. The breathers continue to synchronize until $\delta\omega = \omega_F - \omega_0$ is larger than the frequency window (26), which is field dependent. At this point, $\langle P \rangle$ suddenly drops back to zero. If we use the representative values of TTF-TCNQ as given in RBKT,¹ we find $\Delta\omega/\omega_F = [(1.05 \times 10^{-4}) \alpha E \omega_F / \Gamma]^2$, which for $E = 10^3$ V/cm and $\Gamma \simeq \omega_F$ gives $\Delta\omega/\omega_F \simeq 0.011$, which may be observable. Also note that this frequency window is very sensitive to the values of Γ and α . In particular,

if $\Gamma \simeq 0.1\omega_F$, then $\Delta\omega \simeq \omega_F$ for $E = 10^3$ V/cm, which would certainly be measurable. Thus a measurement of $\Delta\omega$ would be a sensitive measurement of Γ/α .

If the window width is sufficiently small, then one should consider the applied field to contain a distribution of frequencies, in which case $\langle P \rangle$ must be integrated over the entire frequency window in order to calculate the total power absorbed. This step assumes that each breather achieves its synchronous state given by Eqs. (24), independent of the existence of other breather states—an assumption which in a nonlinear system can only be loosely justified by arguing that the effects of cross coupling will average out over time. To estimate the density of breathers n_b , we simply take an estimate from Currie's study of the sine-Gordon model,¹² and let

$$n_b \simeq (\omega_F/c_0) (kT/Mc_0^2), \quad (33)$$

where k is Boltzmann's constant. We shall assume that all of these breathers phase lock with the applied field, and shall ignore any that may be created out of the phonon background. Multiplying Eq. (31) by this factor, integrating over the frequency window, and assuming $\Delta\omega_E \gg \Delta\omega$, where $\Delta\omega_E$ is the bandwidth of the applied field, gives

$$\int n_b \langle P \rangle d\delta\omega = \frac{\alpha \omega_F^2}{12c_0} kT \left(\frac{\omega_F}{\Gamma} \right)^2 \left(\frac{\omega_F}{\Delta\omega_E} \right) \left(\frac{e^* E}{\omega_F M c_0} \right)^3. \quad (34)$$

Using again the representative parameters for TTF-TCNQ and setting $\alpha = G = 1$ (sine-Gordon model), we get for E in V/cm,

$$\int n_b \langle P \rangle d\delta\omega \simeq n_s kT \left(\frac{\omega_F}{\Delta\omega_E} \right) [(5.9 \times 10^{-5}) E]^3. \quad (34')$$

Here we see a strong nonohmic behavior, with the total power absorbed going as E^3 .

The above numerical values suggest that these effects may be observable. The actual physical situation will probably be the broadband case, in which case one should look for a resonance just below ω_F , and for a nonohmic behavior for small fields as given by Eq. (34').

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