The analysis on the single particle model of CDW

Lian-Gang Li, Yong-Feng Ruan

Department of Physics, School of Sciences, Tianjin University, Tianjin 300072, China

Abstract. Grünert put forward a single particle model of charge-density wave, which is a typical nonlinear differential equation, and also a mathematical model of pendulum. This Letter analyzes the solution of equation by the rotated vector fields theory, providing the relation between the applied field \( E \) and the periodic solution, and the conclusion that the critical value of \( E \) for the periodic solution is fixed in the over-damped situation. With these conclusions, it derives the formulae of nonlinear conductivity, narrow-band noise, which are consistent with the empirical ones given by Fleming.

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Keyword: charge-density wave (CDW); pendulum; rotated vector field; periodic solution; narrow-band noise; Grünert’s equation

1. Introduction

Charge-density waves (CDW) is a special phenomenon of electronic condensate in the low dimensional materials and observed in the High Temperature Superconductor materials as well [1]. Many special features associated with CDW, for example, the nonlinear conductivity, narrow-band noise, have been attracting great attention [2–5]. Describing the nonlinear conductivity and narrow-band noise, Grünert and his collaborators proposed a single particle model [6], of which the equation is

\[
\frac{d^2\phi}{dt^2} + \Gamma \frac{d\phi}{dt} + \sin \phi = \beta, \tag{1}
\]

where \( \beta = E/E_0 \) with \( E_0 = (\lambda/2\pi)(m\omega_0^2/e) \) is constant and \( E \) is an electric field applied, \( \Gamma \) is the friction coefficient. Equation (1) is called Grünert’s equation in the CDW theory as well as is the mathematical model of driven, damped pendulum. This is a typical nonlinear differential equation which is non-integrable. In the over-damped situation, Grünert gave an approximate solution with neglect of the inertial term [6]. The derived conductivity, i.e. \( \sigma(E) = \sigma_0 \sqrt{E^2 - E_0^2} \), has an excellent behavior served as the exponent law given in Fleming’s paper in
the region of high field, but this neglect obviously loses some characteristics of original equation, such that it leads to a divergence of the derivative at the threshold field, a intrinsic difference from the experiment result [7].

There are two approaches in the research of nonlinear differential equation. The first one is a classical method which attempts to express the solutions of differential equations into primary functions named closing, or into power series form. This method is difficult to develop further. The second is so-called "the vector field theory of differential equation", originated by Henri Poincaré [8], which treats the solutions as integral curves in the phase space and derives the qualitative properties of the solution geometrically. Many scientists have studied in this theory’s area, such as, G. F. Duff proposed the rotated vector fields in 1953 [9], subsequently, G. Seifert et al. developed it to the general rotated vector fields [10–12].

With general rotated vector fields, this Letter provides some conclusions on the solutions of equation (1), that is, the relation between $\beta$ and the periodic solution, and that, with $\Gamma$ big enough (over damping), the critical value $\beta_0$ will remain unchanged, i.e., $\beta_0 \equiv 1$. Combining these conclusions with the multiple segments model advanced by Portis [13], it derives the same formulae as the empirical ones given by Fleming [7].

2. The periodic solution of the equation

On the $\phi - z$ phase plane, Equation (1) takes the form of vector field:

$$\begin{cases} \frac{d\phi}{dt} = z \\ \frac{dz}{dt} = \beta - \sin \phi - \Gamma z \end{cases},$$

where $\Gamma > 0$, $\beta \geq 0$, whose solutions correspond to the trajectories on the plane. Each trajectory, has a direction running as time goes forward, to which the tangents become vectors which constitute the vector field. When the vectors are rotating owing to the change of some parameter of equation, they constitute the rotated vector field. A point satisfying $\frac{d\phi}{dt} = 0$ and $\frac{dz}{dt} = 0$ is called a "singularity". A field, in which the singularities happen to move accompanying the rotation of vectors, is called the general rotated vector field. In the theory of differential equation, owing to the uniqueness of the solution, the trajectories do not intersect each other except at singularities [14]. This is very useful property in the following analysis.

While $\beta > 1$, there exist no singularities. While $0 \leq \beta \leq 1$, there exist singularities on the $\Phi$-axis with coordinates denoted by $(\phi_n, 0)$ where

$$\begin{cases} \phi_0 = \arcsin \beta \\ \phi_n = n\pi + (-1)^n\phi_0 \end{cases}, \quad n \in \mathbb{Z},$$

which are categorized into two classes, one denoted by $A_k(\phi_{2k-1}, 0)$, the other denoted by $B_k(\phi_{2k}, 0)$, $k \in \mathbb{Z}$. While $\Gamma > 0$, $B_k(\phi_{2k}, 0)$ is called a "focus", which is stable, nearby which all the trajectories spiral into it as time goes forward, as shown in Figure 1 (a). While $\Gamma = 0$, it is called a "center", which is not the subject of the current analysis. $A_k(\phi_{2k-1}, 0)$ is called a "saddle", nearby which there are four trajectories approaching it along two separatrices, as shown in Figure 1 (b). These singularities are key to analyze the equation (2).
For convenience, let $W(\phi, z) = z$, $Q(\phi, z) = \beta - \sin \phi - \Gamma z$. The angle between the vector and the $\Phi$-axis is denoted by $\theta$, where

$$\theta = \tan^{-1} \frac{Q(\phi, z)}{W(\phi, z)}. \tag{4}$$

Clearly, the vector field constructs a rotated vector field when parameter $\Gamma$ or $\beta$ changes. It is different that the singularities do not move as parameter $\Gamma$ changes but move as parameter $\beta$ does, so it is a general rotated vector field with respect to $\beta$. The distribution of vectors is determined by $W(\phi, z)$ and $Q(\phi, z)$, both with a period of $2\pi$ along the $\Phi$-axis, so the vectors distribute with the same period and the plane can be rolled up into a cylindrical surface, that is called a cylindrical system in mathematics. Thus it is enough for analysis that we just discuss the interval $[-\pi - \phi_0, \pi - \phi_0]$ without special declaiming, whereas the others can be extended with periods along the $\Phi$-axis. In the cylindrical system, the trajectory, which connects successive periodic points, will become a cycle on the cylindrical surface, as shown in Figure 2, which is a periodic solution. It is found that equation (2) just possesses such a periodic solution in some condition.

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It is very difficult to tackle the equation (2) directly, but in the case where $\Gamma = 0$ and $\beta = 0$, it offers a simple equation, i.e., $\frac{d^2 \phi}{dt^2} + \sin \phi = 0$, which is called sine-Gordon’s equation, for
which it is easy to give a solution,

\[ z = \sqrt{2(\cos \phi + 1)}. \] (5)

Its corresponding trajectory \( L_0 \) connects saddle point \( A_0 \) with saddle point \( A_1 \), as shown in Figure 3. Point \( A_1 \) is a periodic point of \( A_0 \), so trajectory \( L_0 \) is a cycle on the cylindrical surface, a periodic solution. As connecting two successive saddles, it is called a critical periodic solution in mathematics.

![Figure 3: Trajectories as \( \beta = 0 \)](image)

For which, let \( \Gamma \) increase from zero to a positive, by the analysis of rotated vector field, it is proved that trajectory \( L_0 \) will roll down and become trajectory \( R \) as shown in Figure 3. While \( \Gamma > 0 \), let \( \beta \) increase from zero to a positive value, it is proved that trajectory \( R \) will stretch up and singularity \( A_1 \) moves toward left as well, such that trajectory \( R \) enters singularity \( A_1 \) again at a certain positive value of \( \beta \) which is no greater than 1 [15]. Since point \( A_1 \) is the successive periodic point of \( A_0 \), trajectory \( R \) connecting these two saddles will become a cycle on the cylindrical surface, a critical periodic solution, as shown in Figure 2.

In other words, equation (2) must possess a value \( \beta_0 \) for arbitrary \( \Gamma > 0 \), while \( \beta = \beta_0 \), equation (2) has a critical periodic solution which connects saddle \( A_0 \) with saddle \( A_1 \). By the analysis of rotated vector field, it can also be proved that, while \( \beta \geq \beta_0 \), equation (2) possesses a unique and positive periodic solution, which is stable as well; while \( \beta < \beta_0 \), equation (2) possesses no periodic solution. Through analysis, it shows that \( \beta_0 \) is unique for a given \( \Gamma > 0 \).

According to equation (2), it is easy to obtain

\[ \frac{dz}{d\phi} = \frac{\beta - \sin \phi}{z} \Gamma. \] (6)

On the base of equality (6), it is easy to obtain Theorem 1 as follows.

**Theorem 1.** If a periodic solution \( z = z(\phi) \) exists for the equation (2), i.e., \( z(\phi) = z(\phi + 2\pi) \), \( \phi \in (-\infty, +\infty) \), then it must satisfy

\[ \int_{\phi}^{\phi+2\pi} z(\phi) \, d\phi = \frac{2\pi \beta}{\Gamma}. \] (7)
The proof of Theorem 1 is very simple. According to equality (6), integrating from $\phi$ to $\phi + 2\pi$ and noticing the periodicity of $z(\phi)$, it is easy to obtained equality (7).

According to Theorem 1, it is easy to prove that the periodic solution is unique and positive. In the proof, it just need to notice the property that the trajectories do not intersect each others.

According to the following reason, it is easy to prove that the periodic solution is stable. The periodic solution is a cycle on the cylindrical surface, of which the characteristic exponent is $-\Gamma < 0$, therefore it is a stable limit-cycle [14], a stable periodic solution.

Supposing $\beta_0(\Gamma_1) = 1$ and $\Gamma_2 > \Gamma_1$, it can be proved that, $\beta_0(\Gamma_2) = 1$, that is to say, the critical value $\beta_0$ equals 1 all the time if $\Gamma$ is bigger enough. Interestingly, the slope of $R(\Gamma_2)$ at point $A_1$ is always 0, as shown in Figure 4.

![Figure 4: The critical periodic trajectories as $\Gamma_2 > \Gamma_1$](image)

3. Interpretation of the periodic solution in physics

According to the conclusion above, it follows that while $\beta \geq \beta_0$, Equation (2) must possess a unique, stable and positive periodic solution, where a stable trajectory means that all those nearby will approach it as time goes forward. It indicates that, whatever the initial state it is, the final state will be in a periodic motion toward the positive direction, as shown in Figure 5.

![Figure 5: A stable, positive periodic solution](image)
While $\beta < \beta_0$, Equation (2) possesses no periodic solution. In fact, all trajectories on the phase plane will approach the saddles or foci. If there are some disturbances, they will deviate from the saddles, which are unstable; finally, all the trajectories will end at the foci, which are stable, as shown in Figure 6. In the physics, whatever the initial state it is, the system will stay at equilibrium points (foci) in the stable state.

![Figure 6: Nonperiodic trajectories](image)

Supposing a minimum value $\Gamma_{\text{min}}$ such that $\beta_0(\Gamma_{\text{min}}) = 1$, as above it follows that, while $\Gamma > \Gamma_{\text{min}}$, the critical value $\beta_0$ will be 1 all the time. M. Urabe has given the definite value of it by numerical calculations [16], that is, $\Gamma_{\text{min}} \approx 1.193$. According to the experimental values given in the article [13], $\omega_0 \approx 2\pi \times 210(MHz)$, $\tau = 1.3 \times 10^{-10}(sec)$, $\Gamma = (\omega_0\tau)^{-1}$, it derives $\Gamma = 5.83$. Clearly, in the practical case, $\Gamma$ is greater than $\Gamma_{\text{min}}$ so far so that $\beta_0 = 1$. Because $\beta = E/E_0$, it follows that, while $E \geq E_0$, Equation (1) possesses a unique periodic solution which satisfies Theorem 1, i.e.,

$$2\pi \frac{E}{E_0} = \int_0^{2\pi} \frac{d\phi}{dt} d\phi.$$ (8)

Let $\frac{d\phi}{dt} = \left(\frac{d\phi}{dt}\right)_c + \left(\frac{d\phi}{dt}\right)_a$, where

$$\left(\frac{d\phi}{dt}\right)_c = \frac{E - E_0}{\Gamma E_0},$$ (9)

$$\frac{1}{2\pi} \int_0^{2\pi} \left(\frac{d\phi}{dt}\right)_a d\phi = \frac{1}{\Gamma},$$ (10)

$\left(\frac{d\phi}{dt}\right)_c$ is the uniform velocity of moving as an ensemble and contributing to the direct current conductivity, $\left(\frac{d\phi}{dt}\right)_a$ is the modulated part producing the narrow-band noise. As the difference of velocity between segments results the pressing and stretching each other, the constant component in $\left(\frac{d\phi}{dt}\right)_a$, i.e.

$$\left\langle \left(\frac{d\phi}{dt}\right)_a \right\rangle = \frac{1}{\Gamma},$$ (11)

is turned into energy damage so that no contribution to the current.

4. Application of the multiple segments model

According to the opinions given by Portis [13], the CDWs are pinned by both weak and
strong impurities. The strong impurities, separating the CDW into small segments, are randomly distributed leading to a distribution of separations $l_i$:

$$P(l_i) = \frac{1}{\langle l_i \rangle} e^{-l_i/\langle l_i \rangle}, \quad (12)$$

where $\langle l_i \rangle$ is the mean separation between strong impurities. Each segment is pinned by one strong impurity such that the pinning potential per length acting by strong impurities is $(\langle l_i \rangle / l_i) \sin \phi$. The weak impurities are present in higher concentration such that treated as a constant per length on the average and equivalent to a negative field $E_T$. Thus, the equation for the $l_i$th segment of CDW is expected to be of the form:

$$\frac{d^2 \phi}{dt^2} + \Gamma \frac{d \phi}{dt} + \frac{\langle l_i \rangle}{l_i} \sin \phi = \frac{1}{E_0} (E - E_T), \quad (13)$$

where the friction coefficient $\Gamma$ arises from thermodynamic damping. On the analogy of Equation (1), it derives that when the field $E$ is large than a critical field $E_i$, this segment will slip,

$$E_i = E_T + \frac{l_i}{\langle l_i \rangle} E_0. \quad (14)$$

According to equality (15), it derives that, at a given electric field $E$ there is a critical CDW length $l_E$ such that CDWs longer than $l_E$ are slipping and CDWs shorter than $l_E$ stay at the equilibrium points (i.e. foci) where

$$l_E = \langle l_i \rangle \frac{E_0}{E - E_T}. \quad (15)$$

As all CDWs connect together, integrating Equation (13), it obtains

$$\int_0^{+\infty} \left\{ \frac{d^2 \phi}{dt^2} + \Gamma \frac{d \phi}{dt} + \frac{\langle l_i \rangle}{l_i} \sin \phi \right\} P(l_i) \frac{dl_i}{\langle l_i \rangle} = \int_{l_E}^{+\infty} \left\{ \frac{l_i}{E_0} (E - E_T) - \langle l_i \rangle \sin \phi \right\} P(l_i) \frac{dl_i}{\langle l_i \rangle}. \quad (16)$$

Completing the integral of Equation (16), it obtains

$$\frac{d^2 \phi}{dt^2} + \Gamma \frac{d \phi}{dt} + e^{-E_0/E - E_T} \sin \phi = \frac{1}{E_0} [E_0 + (E - E_T)] e^{-E_0/E - E_T}. \quad (17)$$

Let $v_{CDW}$ denotes the velocity by which the ensemble of CDWs move together, it follows that,

$$v_{CDW} = \frac{\lambda \omega_0}{2\pi} \left( \frac{d\phi}{dt} \right)_e. \quad (18)$$

The factors $\lambda \omega_0 (2\pi)^{-1}$ appear above because Equation (17) is dimensionless and $d\phi/dt$ is a phase velocity. Comparing Equation (17) with (1), it obtains

$$v_{CDW} = \frac{\lambda \omega_0}{2\pi} \frac{1}{\Gamma E_0} (E - E_T) e^{-E_0/E - E_T}. \quad (19)$$

Thus, the conductivity contributed by CDW is

$$\sigma_{DC} = \frac{n e v_{CDW}}{E} = \sigma_0 (1 - \frac{E_T}{E}) e^{-\frac{E_0}{E - E_T}}, \quad (20)$$

where $\sigma_0$ is a measure of the CDW conductivity and $n$ is the concentration of condensed carriers (i.e. CDW). This formula of conductivity is the same as the part contributed by CDW in the Fleming’s empirical ones [7]. Meanwhile, the fundamental frequency of narrow-band noise is

$$f_1 = \frac{v_{CDW}}{\lambda} = \frac{Q}{2\pi n e J_{DC}}, \quad (21)$$
where \( Q \) is the wave vector of CDW, \( J_{DC} \) is the direct current density contributed by CDW. The formula \([21]\), that the fundamental frequency is proportional to the current, is consistent with the result in the article \([7]\), which is postulated on experimental ground.

5. Discussion of Conclusions

The driven damped pendulum is a essential model of nonlinear science \([17, 18]\), which develops many manifestations including chaos and appears in many physical subjects such as the Josephson junctions \([19–21]\). Delicately, the CDW and the Josephson junction, revealing the chaotic behaviors of conducting \([22,23]\), are both well described by the driven damped pendulum model \([24]\). By a rigorous mathematical analysis are derived these conclusions of the pendulum equation applied in \([15]\), which provide us a more direct relation between the pendulum model and the behavior of the CDW. Such a simple model of pendulums indicates us an interesting relations of these physical subjects.

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