Calculation of the Defects Interaction Force with the Ritz Method

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Abstract

The defects are moving with the constant velocity ***V***, on which slow vibrations caused by the interaction is imposed . For very long time nearest-neighbor defects are approaching to each other and then are annihilated. The process of mutual annihilation (confluence) is comparatively fast after the defects have approached close to each other. A single defect frictional force has been found with the help of the Ritz method.

To describe a system with defects the energy functional suggested in [1]has been used :

$$E = -f_0 \sum_k q_k + \int_{-\infty}^{+\infty} (0.5d\phi_x^2 + \Phi(\phi) + \frac{k}{2}\sum_k \delta(x-q_k)\phi^2)dx \qquad (1)$$

Where: $k = 1,...N$; q_k -defect coordinate. To calculate the defect interaction force for the case of a single defect motion the Rirz method has been used.

1. The case when the drawing force f_0 is equal to 0.A single defect structure.

Firstly draw a solution corresponding to a single defect. It is obvious that the solution is even relative to the defect and the defect is stationary. Assume that the defect is isolated at the origin of the coordinate and $\lim \phi(z); \quad z \to \infty$. For the field ϕ we have got:

$$\frac{d}{2}\phi_x^2 - \Phi(\phi) = C_1 \qquad (2)$$

C_+ for all $x > 0$ and C_- for all $x < 0$. Assume that Φ function is equal to 0, for example $\Phi = 0.5\varepsilon\phi^2 + 0.25u\phi^4$. Then, $C_\pm = 0$. Studying (2) at **0** point we have got: $\frac{d}{2}\beta^2 = \Phi(A)$, where:

$$\beta = \phi_x(0^-) = -\phi_x(0^+), \quad \phi(0) = A \tag{3}$$

Studying **0** point singularity we have found $2d\beta = kA$. Finally we have found

$$(kA)^2 = 8d\Phi(A) \tag{4}$$

Amplitude **A** is found from (4). If all powers in $\Phi(A)$ polynomial have positive coefficients , the case is nonlinear and the least power value is equal to 2, then the following existence criterion of the nontrivial solution is :

$$k^2 > 4d\Phi''(0) \tag{5}$$

For the case $\Phi = \frac{1}{2}\varepsilon\Phi^2 + \frac{1}{4}u\Phi^4$ from (5) the following condition for parameter is found : $k > 2\sqrt{\varepsilon d}$. Note, that the ϕ field asymptotic at large distances is as follows:

$$\phi(x) \approx R \cdot \exp(-a|x|), \quad x \to \infty \tag{6}$$

Where $2da^2 = \Phi''(0)$. The obtained solution is denoted by $\eta(x)$. It is clear that if $x = q$, then the equation has the form $\eta(x - q)$.

2. Case $f_0 = 0$. Defects Interaction

Assumed that defects are at large distance from each other, that is $q_1 < q_2 < \ldots < q_N$ and $\min|q_i - q_{i+1}| >> 1$

To apply the Ritz Method approximate solution depending on slow variables q_i should be drawn, substituted into the energy and dissipation expressions and the obtained expressions should be differentiated with respect to q_i *and* dq_i / dt correspondently. Studying the case $\Phi = \frac{1}{2}\varepsilon\phi^2 + \frac{1}{4}u\phi^4$, assume

$$\phi_{appr} = U = \sum_{k=1}^{N} \eta(x - q_k) \tag{7}$$

Substituting this expression into the energy and neglecting translation invariant terms independent on q_k (because their differentiation leads to 0), we have:

$$\overline{E} = E[U] = E_0 + E_1$$

Where:

$$E_0 = \frac{u}{4} \bullet \sum_{k_1,k_2,k_3,k_4}^{i} \int \eta(x - q_{k_1})\eta(x - q_{k_2})\eta(x - q_{k_3})\eta(x - q_{k_4})dx$$

$$E_1 = -\frac{k}{2} \sum_{k,k_2,k_2}^{i} \eta(q_{k_1} - q_{k_2})\eta(q_{k_2} - q_k)$$

(9)

In these sums" I "shows that terms $k_1 = k_2 = k_3 = k_4$ and $k = k_1 = k_2$ are eliminated, because they enter into the translation invariant summand. Study E_1 sum. For each ***k*** terms

$k = k_1, k_2 = k+1, k_2 = k-1,$

$k_2 = k, k_1 = k-1, k_1 = k+1$

make the main contribution.

Assuming that the number of defects is large (N>>1), one can conclude that all contributions are equal. Now it is obvious that:

$$E_1 = -2k\sum_k \eta(q_{k+1} - q_k)\eta(0)$$

Finally:

$$E_1 = -2ARk\sum_k \exp(a(q_k - q_{k+1}))$$

Study sum $\overline{E}_0$. The main contribution to it is made by terms with $k_1 = k_2 = k_3 = k$ and $k_4 = k \pm 1$

Calculation shows

$$\overline{E}_0 \approx -C_1 uR\sum_k \exp(a(q_k - q_{k+1}))$$

where constant $C_1 > 0$ is proportional to integral $\int \exp(az)\eta^3(z)dz$. For the general case this integral is not calculated analytically. For the system behaviour analysis its exact value is not important. Finally:

$$\overline{E}(q) = -R(C_1 u + 2A)\sum_k \exp(a(q_k - q_{k+1}))$$

Then we study the dissipation functional ***D***. We have:

$$D = 0.5\left(\sum_k \left(\frac{dq_k}{dt}\right)^2 + \int \phi_t^2 dx\right)$$

Thus, for large distance between the defects , we have the system of equations which is the parabolic analogy of the Todd chain.

3.Calculation of Single Defect Frictional Force.

Unknown defect velocity is denoted by ***V(t).*** As a matter of fact, it can depend on time. The next approach is applied for small derivative $\frac{dV}{dt}$ (it takes place when the force f_0 is small). Assuming smallness of acceleration the defect structure has the form .$\phi = \phi(x - q(t))$, where $q(t)$- defect coordinate and it is given by the equation (apply the slow surface method or subjection principle):

$$d\phi_{zz} + V\phi_z - \varepsilon\phi - \varepsilon\phi^3 + k\delta(z)\phi = 0$$

Solution ϕ depends on ***V***: $\phi = U(z,V)$. Varying averaged energy with respect to q, we have finally:

$$\frac{dq}{dt} = V = f_0 - 0.5kU(0,V)(U_z(0^+,V) + +U_z(0^-,V))$$

V is found from this equation. From the above the overall conclusion follows ; within the described in this article approximate approaches for a single defect always ***V***= **constant**. It is explained by the fact that the subjection principle describes the steady state condition. The frictional force is

$$F_{\text{lubr}} = -0.5kU(o,V)(U_z(0^+,v) + +U_z(0^-,V))$$

Consider the case when these expressions can be calculated. Asymptotic equations for ϕ at large $|x|$ are :

$$\phi = R_+ \exp(a_+ x),$$

$$x \to +\infty \quad \phi = R_- \exp(a_- x), x \to -\infty$$

where

$$a_\pm = -(2d)^{-1}(V \pm \sqrt{V^2 + 4\varepsilon d})$$

Apply the bifurcation method and find the critical value $k_c(f_0)$ at $f_0 \neq 0$

Let $k = k_c + \tilde{k}$ where $\tilde{k}$ is small. Rewrite the main equation in the form:

$$d\phi_{zz} + V\phi_z - \varepsilon\phi + k_c\delta(z)\phi = u\phi^3 - k\delta(z)\phi$$

(10)

Right part terms are small close to the bifurcation point.

Denote the left part operator as ***L.*** Then the conjugate operator has the form:

$$L^*\phi = d\phi_{zz} - V\phi_z - \varepsilon\phi + k_c\delta(z)\phi$$

Assume that the right part (10) is equal to 0. Then the solution of equation $L\phi = 0$ has the form :

$$\phi_0 = A\exp(a_+ x), x > 0,$$

$$\phi_0 = A\exp(a_- x), \quad x < 0$$

Where $A \neq 0$ if and only if

$$k_c = d(a_+ - a_-) = \sqrt{V^2 + 4\varepsilon d}$$

This relation determines the bifurcation point. At ***k*** less that this critical value the solution of Eq.(10) is trivial.

To find ***A*** amplitude at small $\tilde{k}$, we should note that the eigenfunctions of the conjugate operator L^* are

$$\theta = C_1 \exp(\tilde{a}_+ x), x > 0;$$

$$\theta = \exp(\tilde{a}_- x), x < 0$$

Where:

$$\tilde{a}_{\pm} = -(2d)^{-1}(-V \pm \sqrt{V^2 + 4\varepsilon d})$$

Conclusion

A single defect frictional force has been found with the help of the Ritz method. Qualitative description of the defect system motion is as follows. The defects are moving with the constant velocity ***V***, on which slow vibrations caused by the interaction is imposed . For very long time nearest-neighbor defects are approaching to each other and then are annihilated. The process of mutual annihilation (confluence) is comparatively fast after the defects have approached close to each other. Note here, that the attraction and the approaching of the defects leads to the friction growth, but when the defects have con-flowed, the friction force decreases.

References

1.A.L.Korgenevskii, R.Bausch,RSchmitz, Physical Review Letters V.83,N22,1999,p.4578