Dynamics of dense lattices

Philip Rosenau
Department of Mechanical Engineering, Technion-Israel Institute of Technology, Haifa, 32000, Israel and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
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We derive the equations governing the nonlinear dynamics of one-, two-, and three-dimensional lattices in a close to continuum condition (i.e., a dense lattice). The described method correctly captures all terms to a given order in discreteness and, *unlike* previous approaches, leads to well-behaved partial-differential equations for these problems. In general, the dispersion born out of discreteness counteracts the steepening of waves caused by the nonlinearity and leads to the formation of permanent nonlinear structures.

I. INTRODUCTION

In considering the problem of lattice vibrations one distinguishes two conceptually different spatiotemporal limits. In the first limit the phenomena considered depend crucially on interlattice spacing, e.g., the theory of dislocations. At the other end, which is our main interest here, the characteristic length of the considered phenomena is macroscopic. This scale contains hundreds of not thousands of elementary cells and the natural description of such phenomena appears to be via the continuum approach. While on the continuum level things appear much simpler than on the primordial, discrete level, this simplicity has its price. Firstly, certain long-wave phenomena, as compared with the microscopic unit length, completely disappear. Secondly, the continuum level is described typically by the wave equation

$$y_{tt}=[T(y_x)]_x \ , \tag{1.1}$$

where y and x depending on the model considered, may be scalar or vectors. But quite generally when T is a nonlinear function of its argument, the smooth solution breaks down after a finite time. This is in sharp contrast to the discrete lattice that vibrates smoothly for all times. This catastrophe as predicted by the continuum theory makes it clear that a direct or, should we say, naive approach to continuum leaves out an important effect carried by the discreteness of the system. This effect is, of course, the dispersion borne out of discreteness that is sacrificed when the continuum approach is taken, and it is this dispersion that must be somehow restored in order to counteract the steepening effects caused by the anharmonicity of the interparticle potential. As a first step toward this restoration, consider the vibration of a simple one-dimensional (1D) lattice as given by

$$u_{ntt}=[T(u_{n+1})+T(u_{n-1})-2T(u_n)]/h^2 \ , \tag{1.2}$$

where h is the equilibrium interparticle distance,

$$u_n=\frac{y_n-y_{n-1}}{h} \ ,$$

and y_n is the displacement of the nth particle from equilibrium. Expanding the right-hand side,

$$u_{ntt}\cong[T(u_n)]_{xx}+\frac{h^2}{12}[T(u_n)]_{xxxx}+O(h^4) \ . \tag{1.3}$$

If, following Kruskal and Zabusky,[1] one assumes T to be only weakly nonlinear, setting $u\equiv u_n$ one obtains [up to $O(h^4)$]

$$u_{tt}=[T(u)]_{xx}+\frac{h^2}{12}u_{xxxx} \ , \tag{1.4}$$

and the last term in (1.4) represents the dispersion effects due to discreteness, with h being the trace of the microscopic system. However, the system (1.4) can hardly be considered as a savior from the continuum catastrophe. Firstly, the new term necessitates an additional boundary condition at each end of the chain beyond what is required and supplied by its discrete predecessor. Secondly, the initial-value problem for Eq. (1.4) is ill posed. In fact, with $x\leftrightarrow iK$ and $t\leftrightarrow i\omega$ the dispersion relation for the linearized version of (1.4) reads

$$c^{-2}\omega^2=K^2-\frac{h^2}{12}K^4 \ , \tag{1.5}$$

where c is the speed of sound. And though Eq. (1.4) was derived with long-wave phenomena in mind, short wavelengths are imminently present and will cause the explosion of the solution to Eq. (1.4) in a finite time. One way around the difficulty of properly incorporating the effects caused by discreteness was devised by Kruskal and Zabusky. They further reprocessed Eq. (1.4) by considering only one directional propagation and thus derived (for T being a quadratic function of u) the Korteweg–deVries (KdV) equation. While this approach allowed study and understanding of many phenomena associated with the vibration of a lattice, many other phenomena, like wave-wave interaction, are beyond the realm of the KdV equation.

Our approach outlined next meets the problem head on by regularizing the expansion in the discreteness parameter h. To this end we return to Eq. (1.3) and rewrite it as

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$$u_{tt}=L_A[T(u)]_{xx} \ , \tag{1.6}$$

where

$$L_A=1+\frac{h^2}{12}\partial_x^2+\frac{h^4}{360}\partial_x^4+\cdots \ . \tag{1.7a}$$

Observing that L_A up to $O(h^4)$ is a Schrödinger operator, and thus invertible, we write

$$L_A^{-1}=1-\frac{h^2}{12}\partial_x^2+O(h^4) \ , \tag{1.7b}$$

which when applied to (1.6) yields [up to $O(h^4)$]

$$u_{tt}=[T(u)]_{xx}+\frac{h^2}{12}u_{ttxx} \ , \tag{1.8}$$

which is the desired equation of motion. Note that Eq. (1.8) was derived without any assumption being made on the form of T. The new term in (1.8) is only twice derived in space, thus Eq. (1.8), like its discrete origin or the continuum limit, uses only one boundary condition at each end of the lattice. Its linearized dispersion relation reads

$$c^{-2}\omega^2=\frac{K^2}{1+K^2h^2/12}\rightarrow\begin{cases}K^2(1-K^2h^2/12), & Kh\ll 1\\ 12/h^2, & Kh\gg 1 \ .\end{cases} \tag{1.9a}$$

This should be compared with the dispersion relation of the linearized discrete system that reads

$$c^{-2}\omega^2=\frac{4}{h^2}\sin^2(Kh/2) \ . \tag{1.9b}$$

The standard, direct approach consists of a polynomial expansion of the right-hand side of (1.9b). Such an expansion, however, is meaningful only for finite K. On the other hand, expanding (1.9b) as a rational function, the simplest expression of which is given by the right-hand side of Eq. (1.9a), preserves its boundedness *for all* K. This distinction is crucial because partial-differential equations like Eqs. (1.4) or (1.8), even though derived for small K's actually can be said to employ all K's. And though one does not want to use this high-K part of the information, it is there. It is exactly the blowoff at high K's that ruins Eq. (1.4).

On the contrary, it is the bounded nature of Eq. (1.8) for short wavelengths that makes it a proper tool to study the dynamics of a lattice in a close-to-continuum condition. The dispersion generated by the last term in (1.8) will counteract the steepening caused by the nonlinearity of T, and generate a spatially nonlinear structure of which the solitary wave is the most notable one. For more details regarding this equation, we refer the reader to Refs. 2 and 3.

It is worthwhile at this point to introduce the regularization of the one-sided wave equation namely, the KdV equation. From (1.9b)

$$\pm\omega/c=\frac{2}{h}\sin(Kh/2)$$

$$\cong K-K^3h^2/24\cong\frac{K}{1+K^2h^2/24} \ .$$

The first of these approximations yields the KdV equation, the second its regularization. It is clear that for high K's the KdV equation diverges significantly from its discrete predecessor while the regularized equation preserves its proximity to the original. With this point in mind we derive now the regularized version of the KdV equation. To this end we rewrite Eq. (1.6) as follows:

$$(L_A^{-1/2}\partial_t-\partial_x)(L_A^{-1/2}\partial_t+\partial_x)u=\epsilon[f(u)]_{xx} \ , \tag{1.10a}$$

where

$$T=u+\epsilon f(u), \quad \epsilon\ll 1$$

was assumed to have a dominant linear part and

$$L_A^{-1/2}\cong 1-\frac{h^2}{24}\partial_x^2 O(h^4) \ .$$

Now, since $\epsilon\ll 1$, (1.10a) implies that

$$L_A^{-1/2}\partial_t u\cong\pm\partial_x u \ ,$$

which in turn when properly used in (1.10) and integrated once implies

$$u_t\pm[T^*(u)]_x=\frac{h^2}{24}u_{xxt} \ , \tag{1.10b}$$

where $T^*=u+(\epsilon/2)f(u)$, and $+$ $(-)$ refers to waves propagating to the right (left). Note that for $f(u)=u^2$, Eq. (1.10b) was postulated in Ref. 4 as an approximation that is better than the KdV equation to describe the dynamics of shallow-water waves. In contrast, here this equation is derived in the context of lattice dynamics. In any case the derivation of (1.10b) was not meant to provide a substitute to Eq. (1.8) to which it is inferior on two accounts. Firstly, it describes only a one-sided propagation and secondly, the interparticle potential had to be weakly nonlinear. Rather, it was derived as an alternative to the KdV-type equations, particularly for those cases when the KdV-type equations are not exactly solvable (i.e., when f is neither quadratic nor cubic in u). In a similar fashion in Sec. III, we shall introduce a regularized version of the Kadomtsev-Petviashvili equation (RKP), namely,

$$\partial_x(U_t\pm U_x\pm\alpha U^2U_x-\beta U_{xxt})\pm U_{yy}=0, \quad \alpha,\beta=\text{const} \tag{1.10c}$$

and as before the $+$ $(-)$ sign refers to waves propagating to the right (left).

The main body of this paper is devoted to the application of the regularized expansion method, as outlined above, to one-, two-, and three-dimensional lattices. For the 1D lattice we consider an N-neighbor interaction when the lattice parameters are either homogeneous or inhomogeneous. This is followed by a study of transverse vibration of a 2D lattice without and with periodic substrate potential. Finally, a 3D model due to Batteh and Powell[5] is reconsidered and their equations-of-motion obtained by a direct expansion in h are regularized. We believe that the value of the models presented extend beyond pedagogical interest and will serve to

propagate the use of the presented methodology to study lattice dynamics.

II. 1D LATTICE

A. *N*-neighbor interaction

Consider first the Hamiltonian

$$H=\sum_n\left[\frac{m}{2}\left(\frac{dy_n}{dt}\right)^2+P_1\left(\frac{y_{n+1}-y_n}{h}\right)+P_2\left(\frac{y_{n+2}-y_n}{2h}\right)\right],$$

which describes the interaction between two closest neighbors with h being the equilibrium spacing between two adjacent point masses [see Fig. (1)], and P_i $(i=1,2)$ being the interaction potentials. The equations of motion are

$$h\rho_0\frac{d^2y_n}{dt^2}=\left[T_1\left(\frac{y_{n+1}-y_n}{h}\right)-T_1\left(\frac{y_n-y_{n-1}}{h}\right)\right]+\tfrac{1}{2}\left[T_2\left(\frac{y_{n+2}-y_n}{2h}\right)-T_2\left(\frac{y_n-y_{n-2}}{2h}\right)\right], \tag{2.1}$$

where $T_i=\partial_u P_i(u)/h$, $i=1,2$, is the tension function and $\rho_0=m/h$ is the uniform density of the continuum. Unlike the first neighbor-interaction problem, in what follows it is necessary to assume that T_i has a dominant linear part (i.e., it is weakly nonlinear), i.e.,

$$\frac{1}{\rho_0}T_i(u)=C_i^2u+h_i^{\alpha_i}f_i(u),\quad 0<\alpha_i,\ i=1,2\ . \tag{2.2}$$

The actual form of f is assumed to be known but need not be stated. The right-hand side of (2.1) is now Taylor expanded around y_n to obtain $(y\equiv y_n)$

$$y_{tt}=L_1[T_1]_x+L_2[T_2]_x+O(h^{2+\alpha_1}+h^{2+\alpha_2})\ , \tag{2.3}$$

here

$$T_i=T_i(y_x),\quad i=1,2$$

and

$$L_i=1+\frac{2(ih)^2}{4!}\partial_x^2+\frac{2(ih)^4}{6!}\partial_x^4+\cdots,\quad i=1,2\ . \tag{2.4}$$

In what follows the index n will be dropped. Now we have two operators L_1 and L_2 as candidates for inversion if the procedure outlined in the introduction is to be repeated. Actually there appear to be infinitely many ways to blend h_1 and h_2 and invert them. The one selected is chosen requiring consistency in the sense that the present problem should reduce to the basic lattice (i.e., interaction with adjacent neighbors only) described in the introduction if second-neighbor interaction vanishes. To this end define

$$L_A=\beta_1L_1+\beta_2L_2\cong 1+\frac{\gamma_2h^2}{12}\partial_x^2+O(h^4)\ , \tag{2.5a}$$

where

$$\beta_i=\frac{C_i^2}{C_1^2+C_2^2},\quad i=1,2 \tag{2.5b}$$

$$\gamma_2=S_0/(C_1^2+C_2^2),\quad S_0=C_1^2+4C_2^2\ . \tag{2.5c}$$

As before, L_A, up to $O(h^4)$, is a Schrödinger operator. Thus, Eq. (2.3) reads

$$y_{tt}=L_Ay_{xx}+h^{\alpha_1}L_1[f_1(y_x)]_x+h^{\alpha_2}L_2[f_2(y_x)]_x+O(h^{2+\alpha_1}+h^{2+\alpha_1})\ . \tag{2.6}$$

Acting with L_A^{-1} we then have [up to $O(h^{2+\alpha_1}+h^{2+\alpha_2})$]

$$y_{tt}=[T_1(y_x)+T_2(y_x)]_x+\frac{\gamma_2h^2}{12}y_{xxtt}\ , \tag{2.7}$$

which is the desired equation of motion. Note that the direct expansion would yield

$$y_{tt}=[T_1(y_x)+T_2(y_x)]_x+\frac{h^2S_0}{12}y_{xxxx}\ . \tag{2.8}$$

An equation of this type was, for instance, derived by Peyrard, Pnevmatikos, and Flytzanis (c.f. Ref. 6 and references therein). As in the case of the first-neighbor interaction, an initial-value problem cannot be properly posed for Eq. (2.8). We note also that the present results are somehow weaker than the one obtained for the one-neighbor interaction. Because we had to invert both L_1 and L_2 we had to assume that T_i is weakly nonlinear. Equation (2.7) has formally the same form as Eq. (1.8) but with an effectively new tension function and an enhanced effect of dispersion. Note also that Eq. (2.7) is derivable from a Lagrangian density $\mathcal{L}$ where

$$\mathcal{L}=\tfrac{1}{2}y_t^2-P_*(y_x)+\frac{h^2\gamma_2}{24}(y_{xt})^2\ , \tag{2.9}$$

and $P_*=P_1(y_x)+P_2(y_x)$. Equation (2.7), similarly to Eq. (1.8), has as pointed out in Ref. 2, a finite number of conservation laws.

Generalization to a mass point interacting with N neighbors presents no difficulty. Let $i=1,\ldots,N$; then defining

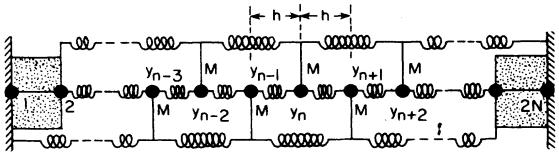

FIG. 1. A Schematic diagram of a 1D lattice with a two-neighbor interaction.

$$C_N^2=\sum_{j=1}^{N} C_j^2,\quad \beta_j=C_j^2/C_N^2,\quad \gamma_N=\sum_{j=1}^{N} j^2\beta_j\ , \tag{2.10a}$$

and

$$L_A=\sum_{j=1}^{N}\beta_j L_j\cong 1+\gamma_N h^2\partial_x^2+O(h^4)\ , \tag{2.10b}$$

we have

$$y_{tt}=\left[\sum_{j=1}^{N} T_j(y_x)\right]_x+h^2\frac{\gamma_N}{12}y_{xxtt}\ . \tag{2.10c}$$

Notice that the increase in N causes both the increase of γ_N and C_N^2. γ_N is the effective measure of the overall dispersion while C_N^2 gives the effective acoustic speed. If all C are equal, $C_i\equiv C_*$, $\forall i$, then $C_N=NC_*$ and the ratio

$$d_*=\gamma_N/N=\sum_{j=1}^{N}\left[\frac{j}{N}\right]^2$$

measures the effective increase in dispersion with the increase in the number of interacting neighbors. As N varies from 1 to 5, d_* varies from 1.1 to 2.2.

It is of interest to point out that in Ref. 6 where Eq. (2.8) was derived, S_0 (h_0 in their notation) was taken to be both positive and negative. A negative value of S_0 was achieved when an inverted potential for the interaction with the second neighbors was used. Now while Eq. (2.8) is ill posed for $S_0>0$, it is a perfectly well-defined mathematical object for $S_0<0$. However, in spite of being well posed even for $S_0<0$, Eq. (2.8) poorly approximates its discrete predecessor. Indeed for $S_0<0$, the dispersion relation of (2.8) yields

$$\omega^2=(C_1^2+C_2^2)K^2+|S_0|K^4\ .$$

By assumption,

$$C_2^2+C_1^2>0,\quad S_0\equiv C_1^2+4C_2^2<0\ ,$$

which predicts that for large K, $\omega\sim\pm K^2$ and $K\nearrow\infty\rightarrow\omega\nearrow\infty$. But the original, discrete version gives

$$\omega^2=[4C_1^2\sin^2(Kh/2)+C_2^2\sin^2(Kh)]/h^2$$

$$=\frac{4}{h^2}\sin^2(Kh/2)[C_1^2+C_2^2\cos^2(Kh/2)]\geq 0\ . \tag{2.11}$$

Evidently, in (2.11) ω is bounded for all K's. Thus the high K content is completely misrepresented.

Resolution of this somehow esoteric case is more complicated because $S_0<0\rightarrow\gamma_2<0$ [see Eq. (2.5c)] making our expansion in rational functions "as is" invalid. To see how to resolve this difficulty we expand the right-hand side of (2.11) as follows:

$$\omega^2=(C_1^2+C_2^2)K^2-(C_1^2+4C_2^2)h^2K^4/12+O(K^6h^4) \tag{2.12a}$$

$$=\frac{(C_1^2+C_2^2)K^2}{1+\gamma_2(Kh)^2/12}+O(K^6h^4)\ . \tag{2.12b}$$

It is clear that for $\gamma_2<0$ the expression in rational functions cannot be terminated at the quadratic level, as was done in all previous cases, and must be continued to the next, quartic level. The simplest such expression, when sixth order in (2.12a) is included, is

$$\omega^2=A_0K^2+A_1K^4-A_2K^6=\frac{A_0K^2+A_1K^4}{1+K^4A_2/A_0}\ ,$$

$$A_0,A_1,A_2>0\ ,$$

where $A_0=C_1^2+C_2^2$, $A_1=-(C_1^2+4C_2^2)h^2/12$, [compare with Eq. (2.12a)] and $A_2=-(C_1^2+16C_2^2)h^4/360$. (In Ref. 6 it was assumed that $C_1^2=1$ and $C_2^2=-0.4$. Thus $A_0=0.6$, $A_1=0.05h^2$, and $A_2=0.015h^4$.) The resulting differential equation

$$y_{tt}=[T_1(y_x)+T_2(y_x)]_x-A_1y_{xxxx}-\frac{A_2}{A_0}y_{xxxxtt} \tag{2.12c}$$

has an additional, sixth-order term.

This case will not be persued further. It was brought forth mainly to illuminate the necessity of a careful examination of the relations between the discrete and the quasicontinuous level.

B. Inhomogeneous lattice

In this section we derive the equations governing the propagation of waves along one-dimensional inhomogeneous lattice. It will be assumed that the variation of the parameters is of the order of the variation due to the discreteness. We start with the one-neighbor-interaction case. Generalization to N interacting neighbors will follow. It is also convenient to start with a concrete potential. We take

$$\begin{aligned} m_n\ddot{y}_n=&K_{n+1}[(y_{n+1}-y_n)/h\\ &+A_{n+1}(y_{n+1}-y_n)^{\omega+1}/h^{\omega+1}]\\ &-K_n[(y_n-y_{n-1})/h+A_n(y_n-y_{n-1})^{\omega+1}/h^{\omega+1}]\ , \end{aligned} \tag{2.13}$$

m_n and y_n are the mass of the nth particle and its displacement from equilibrium, respectively. A_n measures the relative strength of the anharmonic force acting on the nth particle and ω is a positive constant. We assume that the variable parameters are expandable as follows:

$$\begin{bmatrix} m\\ K\\ A\end{bmatrix}_{n+1}=\begin{bmatrix} m\\ K\\ A\end{bmatrix}_n+h\frac{d}{dx}\begin{bmatrix} m\\ K\\ A\end{bmatrix}_n+O(h^2)\ . \tag{2.14}$$

The slowness of variation of our parameters will be explicitly introduced as

$$\begin{aligned} &\rho(x)=m/h=\rho^0[1+hM(x)],\quad M=O(1)\\ &K=K^0[1+h^{1+\alpha}S(x)],\quad S=O(1),\quad \alpha=\text{const}\\ &A=A^0[h^{\omega}+h^{1+\omega}a(x)],\quad a=O(1)\ , \end{aligned} \tag{2.15}$$

where ρ^0, K^0, and A^0 are constants. We now expand in the usual fashion, act with the operator L_A^{-1}, drop the index n, and obtain up to $O(h^2)$

$$\rho(x)y_{tt}=\{K(x)[1+A(x)y_x^{\omega}]y_x\}_x + \frac{h^2\rho(x)}{12}y_{xxtt}+\frac{h^{2+\alpha}}{2}K^0(S_xy_x)_x \ . \quad (2.16a)$$

Clearly, if $\alpha>0$, the last term in (2.16a) may be dropped. But if $\alpha=0$, inhomogeneity causes the explicit appearance of an additional term that disappears only in the homogeneous case. Thus, for $\alpha=0$ we may write (2.16a) as

$$\rho(x)y_{tt}=\left[K(x)\left[1+\frac{h}{2}(\ln K)_x+A(x)y_x^{\omega}\right]y_x\right]_x + \frac{h^2\rho(x)}{12}y_{xxtt} \ . \quad (2.16b)$$

Clearly, inhomogeneity and discreteness combined modify the effective tension of the lattice. Now from Eqs. (2.16) generalization to an arbitrary weakly anharmonic tension T is obvious. It is easy to generalize formula (2.16b) to the case of N interacting neighbors. We obtain

$$R(x)y_{tt}=\sum_{j=1}^{N}\left[\tilde{T}_j(y_x)+\frac{h}{2}(c_j^2)_xy_x\right]_x + R(x)\frac{\gamma_N}{12}y_{xxtt} \ , \quad (2.17)$$

where

$$R(x)=\rho/\rho^0=1+hM(x) \ , \quad (2.18a)$$

$$c_j^2=K_j/\rho^0=[1+hS_j(x)](c_j^0)^2, \quad (c_j^0)^2=K_j^0/\rho^0 \quad (2.18b)$$

$$\tilde{T}_j(y_x)=c_j^2y_x+h^{\omega_j}f(y_x), \quad \omega_j>0 \quad (2.18c)$$

and γ_N similarly to (2.10a) is given as

$$\gamma_N=\sum_{j=1}^{N}j^2\beta_j, \quad \beta_j=(c_j^0)^2/c_N^2, \quad c_N^2=\sum_{j=1}^{N}(c_j^0)^2 \ . \quad (2.18d)$$

A nonregularized version of Eqs. (2.16), with a random inhomogeneity, was presented in Ref. 7.

III. 2D LATTICE: THE CASE OF TRANSVERSE VIBRATIONS

A. Analysis

Consider a 2D rectangular lattice of mass points as shown on Fig. 2(a). We assume that the lattice is free to execute a small but finite motion in a transverse (i.e., z) direction to its initial position in the x-y plane. Consider a balance of forces of a typical mass element of the lattice located at the (m,n) site of the lattice as shown in Fig. 2(b). We have

$$m\frac{d^2}{dt^2}Z_{m,n}=[(\mathbf{F}_{m+1,n}+\mathbf{F}_{m-1,n}) + (\mathbf{F}_{m,n-1}+\mathbf{F}_{m,n+1})]\cdot\mathbf{e}_z \ . \quad (3.1)$$

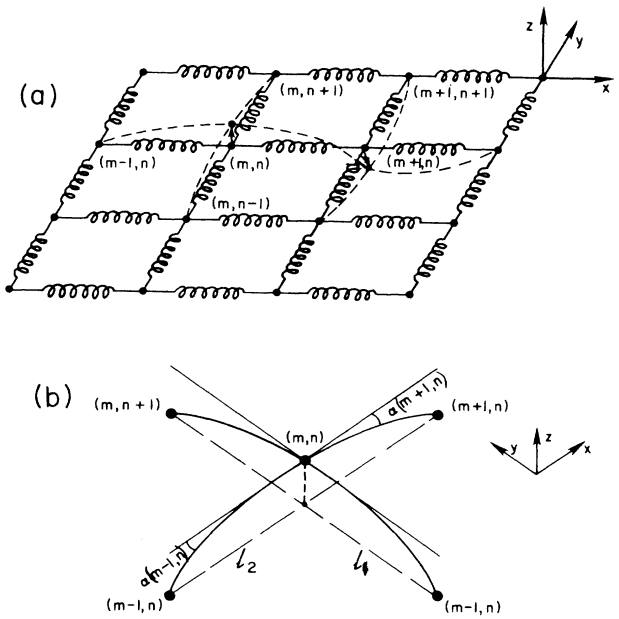

FIG. 2. (a) A 2D lattice in the (x,y) plane. The lattice is assumed to vibrate in direction perpendicular to its planar position. (b) Perpendicular displacement of a typical (m,n) mass point from its equilibrium position.

We study each part of the forces separately,

$$F_{m,n\pm1}=\pm\left[T_1+K_1l_1\left[\frac{1}{\cos\alpha_{m,n\pm1}}-1\right]\right]\sin\alpha_{m,n\pm1} \ , \quad (3.2)$$

where T_1 is the tension of the springs in equilibrium in y direction of the originally prestretched lattice, K_1 is their elastic constant, and α is the local angle between the lattice and the y axis. Assuming α to be small we have up to third order in α

$$F_{m,n\pm1}=\pm\left[\frac{T_1}{l_1}+\frac{K_1l_1-T_1}{2l_1^3}(\Delta Z_{n\pm1})^2\right]\Delta Z_{n\pm1} \ , \quad (3.3a)$$

where

$$\Delta Z_{n\pm1}\equiv\pm(Z_{m,n\pm1}-Z_{m,n}) \ .$$

Similarly in the x direction we have

$$F_{m\pm1,n}=\pm\left[\frac{T_2}{l_2}+\frac{K_2l_2-T_2}{2l_2^3}(\Delta Z_{m\pm1})^2\right]\Delta Z_{m\pm1} \ , \quad (3.3b)$$

where

$$\Delta Z_{m\pm1}\equiv\pm(Z_{m\pm1,n}-Z_{m,n}) \ , \quad (3.4)$$

and T_2 and K_2 are the equilibrium tension and elastic constant, respectively, in the x direction. Thus

$$m\frac{d^2}{dt^2}Z=\left[\frac{T_1}{l_1}+A_1(Z_{m,n+1}-Z_{m,n})^2\right](Z_{m,n+1}-Z_{m,n})-\left[\frac{T_1}{l_1}+A_1(Z_{m,n}-Z_{m,n-1})^2\right](Z_{m,n}-Z_{m,n-1})$$
$$+\left[\frac{T_2}{l_2}+A_2(Z_{m+1,n}-Z_{m,n})^2\right](Z_{m+1,n}-Z_{m,n})-\left[\frac{T_2}{l_2}+A_2(Z_{m,n}-Z_{m-1,n})\right](Z_{m,n}-Z_{m-1,n}) , \tag{3.5}$$

where

$$A_i=\frac{K_i l_i-T_i}{2l_i^3},\quad i=1,2 .$$

Expanding $Z_{m\pm1,n}$ and $Z_{m,n\pm1}$ around $Z_{m,n}$ we obtain

$$\frac{\partial^2 Z_{m,n}}{\partial t^2}=L_y\frac{\partial^2 Z_{m,n}}{\partial y^2}\left[C_1^2+\sigma_1\left[\frac{\partial Z_{m,n}}{\partial y}\right]^2\right]$$
$$+L_x\frac{\partial^2 Z_{m,n}}{\partial x^2}\left[C_2^2+\sigma_2\left[\frac{\partial Z_{m,n}}{\partial x}\right]^2\right] , \tag{3.6}$$

where

$$\sigma_i=\frac{3}{2}\left[\frac{K_i l_i}{m}-C_i^2\right],\quad C_i^2=\frac{T_i l_i}{m},\quad i=1,2 \tag{3.7}$$

and

$$L_y=1+\frac{l_1^2}{12}\frac{\partial^2}{\partial y^2}+\frac{2}{6!}l_1^4\frac{\partial^4}{\partial y^4}+\cdots ,$$
$$L_x=1+\frac{l_2^2}{12}\frac{\partial^2}{\partial x^2}+\frac{2}{6!}l_2^4\frac{\partial^4}{\partial x^4}+\cdots . \tag{3.8}$$

As in the one-dimensional case, a direct use of L_x and L_y renders the problem ill posed. Exploiting the assumption of weak nonlinearity of the system, we invert both L_x and L_y and note that

$$L_A^{-1}=(L_xL_y)^{-1}=L_x^{-1}L_y^{-1}=L_y^{-1}L_x^{-1}$$
$$\cong 1-\tfrac{1}{12}(l_1^2\partial_y^2+l_2^2\partial_x^2)+\tfrac{1}{144}l_1^2l_2^2\partial_x^2\partial_y^2+O(l_1^4+l_2^4) . \tag{3.9}$$

The last retained operator term, though formally of higher order, is of mixed nature and its use does not necessitate an imposition of additional boundary conditions beyond what is required by the lower-order terms. As we shall see, this term will be needed to derive a model consistent with its discrete predecessor. Now acting with L_A^{-1} on Eq. (3.6) and denoting $Z\equiv Z_{m,n}$, we have

$$\frac{\partial^2 Z}{\partial t^2}=\left[C_1^2+\sigma_1\left[\frac{\partial Z}{\partial y}\right]^2\right]\frac{\partial^2 Z}{\partial y^2}+\left[C_2^2+\sigma_2\left[\frac{\partial Z}{\partial x}\right]^2\right]\frac{\partial^2 Z}{\partial x^2}$$
$$+\frac{1}{12}\left[l_1^2\frac{\partial^2}{\partial y^2}+l_2^2\frac{\partial^2}{\partial x^2}\right]\frac{\partial^2 Z}{\partial t^2}$$
$$-\tfrac{1}{144}l_1^2l_2^2\frac{\partial^6 Z}{\partial x^2\partial y^2\partial t^2}-\tfrac{1}{12}(C_1^2l_2^2+C_2^2l_1^2)\frac{\partial^4 Z}{\partial x^2\partial y^2} . \tag{3.10}$$

In the important subcase of an isotropic lattice, the last equation simplifies somehow and we have ($C=C_1=C_2$, $l=l_1=l_2$)

$$\frac{\partial^2 Z}{\partial t^2}=\mathrm{div}[(C^2+\sigma\,|\,\nabla Z\,|^2)\nabla Z]+\frac{l^2}{12}\nabla^2\frac{\partial^2 Z}{\partial t^2}$$
$$-\frac{l^2C^2}{6}\frac{\partial^4 Z}{\partial x^2\partial y^2}-\frac{l^4}{144}\frac{\partial^6 Z}{\partial x^2\partial y^2\partial t^2} . \tag{3.11}$$

The memory of the discrete structure is carried by Eqs. (3.10) and (3.11) in two ways. Firstly, there is the microscopic characteristic length; secondly, the last two terms in Eqs. (3.10) and (3.11), like their discrete predecessor, are noninvariant under infinitesimal rotation. Since the first three terms of Eq. (3.11) have an invariant form, it seems advantageous to drop the invariance-breaking terms and to study

$$\frac{\partial^2 Z}{\partial t^2}=\mathrm{div}[(C^2+\sigma\,|\,\nabla Z\,|^2\nabla Z]+\frac{l^2}{12}\nabla^2\frac{\partial^2 Z}{\partial t^2} . \tag{3.12}$$

Since the main impact of the neglected terms is dispersive, we pause to compare the various dispersion relations. For (3.11) the linearized version yields

$$\frac{\omega^2}{C^2}=\frac{K^2+l^2K_x^2K_y^2/6}{1+l^2K^2/12+l^4K_x^2K_y^2/144}$$
$$=\frac{K_x^2}{1+K_x^2l^2/12}+\frac{K_y^2}{1+K_y^2l^2/12} , \tag{3.13}$$

while for (3.12) we have

$$\frac{\omega^2}{C^2}=\frac{K^2}{1+l^2K^2/12},\quad K^2=K_x^2+K_y^2 . \tag{3.14}$$

Like in the 1D case, we compare these results with the linearized discrete version. For the discrete isotropic case we have

$$\frac{\omega^2}{C^2}=\frac{4}{l^2}[\sin^2(K_xl/2)+\sin^2(K_yl/2)] \tag{3.15}$$
$$\cong\frac{K_x^2}{1+K_x^2l^2/12}+\frac{K_y^2}{1+K_y^2l^2/12}+O(K^6) . \tag{3.16}$$

Comparing (3.13) with (3.16) we see that to a needed accuracy Eq. (3.11) indeed reproduces faithfully the dispersive effects due to the discreteness. While Eq. (3.12) is slightly less accurate [compare (3.14) with (3.13)] it varies meaningfully from (3.11) only when both K_x and K_y are very large, a wavelength domain in which we do not expect anyway a great accuracy from a quasicontinuum theory. In lieu of its simplicity Eq. (3.12) seems more amenable to analysis than Eq. (3.11). We shall

therefore adopt (3.12) as the quasicontinuous model of the lattice. In passing, we note that to obtain a proper dispersive balance both (or none) of the $K_x^2K_y^2$ terms in (3.13) are needed. That is why the fourth-order term in the expansion of L_A^{-1} was originally retained; it was needed to balance comparable terms coming from the action of L_A^{-1} on L_y and L_x, respectively.

Making Eq. (3.12) our prime object of interest we note that it is derivable from a Lagrangian density

$$\mathcal{L}=\frac{1}{2}\left[\frac{\partial Z}{\partial t}\right]^2-\frac{C^2}{2}|\nabla Z|^2-\frac{\sigma}{3}|\nabla Z|^3+\frac{l^2}{24}|\nabla Z_t|^2 . \tag{3.17}$$

Multiplying Eq. (3.12) by 1, t, Z_t, ∇Z, and Z_θ, respectively, and integrating by parts we have

$$\int_{\partial\Omega} Z_t d\Omega=I_1, \quad \int_{\partial\Omega} Z\, d\Omega=I_1 t+I_2 , \tag{3.18a}$$

$$\int_{\partial\Omega}\left[\frac{1}{2}(Z_t^2+C^2|\nabla Z|^2)+\frac{\sigma}{3}|\nabla Z|^3+\frac{l^2}{24}|\nabla Z_t|^2\right]d\Omega=I_3 , \tag{3.18b}$$

$$\int_{\partial\Omega}\nabla Z\left[Z_t-\frac{l^2}{12}\nabla^2 Z_t\right]d\Omega=\underline{I}_4 , \tag{3.18c}$$

$$\int_{\partial\Omega} Z_\theta\left[Z_t-\frac{l^2}{12}\nabla^2 Z_t\right]d\Omega=I_5 , \tag{3.18d}$$

where

$$I_2=\int_{\partial\Omega} Z(x,y,t=0)d\Omega, \quad Z_\theta\equiv xZ_y-yZ_x ,$$

and it is assumed that the contribution of surface integrals has vanished. The first and the third constants of motion have a clear physical meaning; the first represents the conservation of linear momentum and the third, the conservation of energy. No further conservation laws are known to us at this time.

Note that Eq. (3.12) supports a one-dimensional traveling wave. Let

$$\zeta=\mathbf{K}\cdot\mathbf{r}-\Omega(|\mathbf{K}|)t , \tag{3.19}$$

then (3.12) yields [$R=Z'(\zeta)$]

$$\frac{l^2}{12}K^2\Omega^2R''+(K^2C^2-\Omega^2)R+\sigma K^4R^3=0 , \tag{3.20}$$

which has a solitary-wave solution

$$R=\pm\frac{\sqrt{3}}{|\mathbf{K}|}\hat{S}\,\mathrm{sech}\left[\hat{S}\left(\frac{\sqrt{12}}{l\Omega}\mathbf{K}\cdot\mathbf{r}-\hat{S}^2t+r_0\right)\right] ,$$

$$r_0=\text{const}$$

and

$$\hat{S}^2=\Omega-K^2C^2\geq 0 \tag{3.21}$$

is a constant.

B. A weakly-dependent 2D system

We consider the intermediary case between the dynamics of 1D and 2D lattices, wherein the changes in the, say, y direction may be assumed to be slow. We introduce

$$\eta=ly/C \tag{3.22a}$$

and assume that $Z=0(l)$ or alternatively $\sigma=l^2\bar{\sigma}$. Let also

$$s=x-Ct \quad \text{and} \quad \tau=\frac{l^2t}{2C} , \tag{3.22b}$$

then

$$\frac{\partial^2 Z}{\partial\tau\partial s}+\frac{\partial}{\partial s}\left[\sigma\left[\frac{\partial Z}{\partial s}\right]^2\frac{\partial Z}{\partial s}\right]+\frac{\partial^2 Z}{\partial\eta^2}+\frac{1}{12}\frac{\partial^4 Z}{\partial s^4}=0 ; \tag{3.23}$$

in terms of $A=\partial_s Z$ we have

$$\frac{\partial}{\partial s}\left[\frac{\partial A}{\partial\tau}+\sigma\frac{\partial}{\partial s}A^3+\frac{1}{12}\frac{\partial^3 A}{\partial s^3}\right]+\frac{\partial^2 A}{\partial\eta^2}=0 , \tag{3.24}$$

which is the cubic version of the (quadratic) Kadomtsev-Petviashvili (KP) equation. Clearly, if the slow variation in the y direction is completely suppressed, Eq. (3.24) becomes the modified KdV equation which describes transverse vibration of a 1D lattice. Unlike the KP equation, Eq. (3.24) does not seem to be exactly integrable. Further study is needed to assess its properties.

In addition to its nonintegrability (integrability is, after all, the main asset of the KP equation) the modified KP, Eq. (3.24), like the KP itself, for high K's, poorly approximates the original system. Thus we reapply the procedure used for the regularization of the KdV equation. To this end we use Eq. (3.22a) in (3.6) to obtain up to $O(l^4)$

$$Z_{tt}=L_x(C^2+\sigma Z_x^2)Z_{xx}+l^2Z_{yy}$$

or

$$(L_x^{-1/2}\partial_t-C\partial_x)(L_x^{-1/2}\partial_t+C\partial_x)Z=l^2(\bar{\sigma}Z_x^2Z_{xx}+Z_{yy}) ,$$

and only the isotropic case is considered. Since the right-hand side of the last expression is $O(l^2)$, we assume that

$$L_x^{-1/2}\partial_t\cong\pm C\partial_x$$

to obtain after proper substitution of this approximation and $U=Z_x$

$$U_t\pm\left[CU+\frac{\epsilon\bar{\sigma}}{3}U^3\right]_x\pm\epsilon\partial_x^{-1}U_{yy}=\frac{\epsilon C}{12}U_{xxt} ,$$

$$\epsilon=l^2/2C \tag{3.25}$$

which is the desired equation of motion. The $+$ ($-$) sign refers to propagation to the right (left). It is Eq. (3.25) that should be used to study the one-sided propagation of waves in a weakly 2D system.

C. Substrate potential

Recently, the two-dimensional Sine-Gordon (SG) system has been extensively studied[8] in connection with wide applicability to realistic physical systems such as an adsorbed monolayer.[9] A typical Hamiltonian adopted for such studies is[10]

$$H=\tfrac{1}{2}\sum_{i,j}\{\dot{Z}_{i,j}^2+(Z_{i+1,j}-Z_{i,j})^2 +\gamma(Z_{i,j+1}-Z_{i,j})^2+V_0[1-\cos(2\pi x_{i,j})]\}\ .$$

V_0 is the amplitude of the periodic potential and γ is the anisotropic parameter. As pointed by us for the one-dimensional case[2] there is no physical reason why the anharmonic part of the interparticle potential should be neglected. Differently stated, motion due to the substrate potential will evoke a nonharmonic part of the interparticle potential. This neglect appears to be rather a matter of habit than reason. A detailed derivation for the 1D system with arbitrary periodic and interparticle potentials was given in Ref. 2. Using the results of Sec. III A we generalize the harmonic (SG) 2D system to a 2D weakly nonharmonic system with an arbitrary substrate potential. Combining the results of Ref. 2 and Sec. III A we obtain for the rectangular lattice [c.f. Eq. (3.12)]

$$\frac{\partial^2 Z}{\partial t^2}=\mathrm{div}\left[\left[C^2+\sigma\,|\,\nabla Z\,|^2-\frac{l^2}{12}V'(Z)\right]\nabla Z\right] +V(Z)+\frac{l^2}{12}\nabla^2\frac{\partial^2 Z}{\partial t^2}\ , \tag{3.26}$$

where $V(Z)$ is an arbitrary periodic function.

One observes the appearance of two new terms as compared with the harmonic (SG) case. The first term which modifies the effective tension by $-l^2V'(Z)/12$ prevents (3.26) from being derivable from a Lagrangian. Since V is a bounded function this term is always small compared with the linear part, and unlike the anharmonic part $\sigma\,|\,\nabla Z\,|^2$, its contribution to the effective speed of sound can never become important. *Henceforth,* it will be *neglected.* Note, however, that with neglect of this term, discreteness will have an impact only on the dynamics of the systems; the equilibrium is that of the continuum. Now the last term in (3.26) is new in the SG context. Whether the periodic substrate potential is present or not, *once the anharmonic forces have been included,* the system will proceed to catastrophe (unbounded growth of gradients, loss of smoothness, and thus a solution that ceases to exist in the classical sense) unless counteracted by dispersion induced by the discreteness. In the standard (SG) formulation nonharmonic interparticle processes are totally excluded, thus one can proceed to continuum. While effects due to discreteness are known to modify the continuum theory, this theory in the harmonic case can stand on its own, as is. The addition of nonharmonic forces, even if small, dramatically changes this picture. One cannot proceed to continuum directly because the periodic potential is incapable of arresting the formation of singularities. It is here that discreteness becomes essential. In a way, in Eq. (3.26) a balance is created between two pairs of forces; the harmonic forces balance the periodic force V, while the anharmonic part is balanced by the dispersion. This competition suggests the existence of a far richer structure than in the harmonic SG case.

IV. WAVES IN A THREE-DIMENSIONAL LATTICE

In this section we will be concerned with deriving the equations of motion governing the propagation of disturbances in a face-centered-cubic (fcc) lattice in close-to-continuum conditions. In the choice of the specific parameters we follow the work of Batteh and Powell[5] that assumed the atoms of the lattice to interact via a Morse-type interatomic potential. The part of their work that is concerned with the derivation of equations of motion in near-to-continuum conditions suffers from the usual shortcoming caused by the direct expansion in the discreteness parameter. We stress again that while such equations can be used to calculate solitary waves their equations *cannot* be used to study the dynamics or interaction of such waves.

Before presenting the resulting regularized equations, we summarize the assumptions leading to their derivation: (a) Only nearest-neighbor interactions are included, (b) the fcc lattice is unbounded in the z direction and is periodic in the x and y directions, and (c) we will be concerned only with planar oscillations; each atom in a plane normal to the z direction will be assumed to have the same velocity and displacement. The velocities and displacements have a y component (transverse) and a z component (longitudinal), but for simplicity, the x components will be set equal to zero. Now let $\mathbf{S}_K$ stand for the displacement of plane K from its equilibrium position. Noting that each point interacts with 12 neighbors, and expanding the discrete equations of motion with the Morse potential through second order in S, we have (for more details see Ref. 5 pp. 1403 and 1404)

$$(\ddot{S}_K)_y=4R^2\{(S_{K+1}+S_{K-1}-2S_K)_y +(1-3R)[(S_{K+1}-S_K)_y(S_{K+1}-s_K)_z-(S_{K-1}-S_K)_y(S_{K-1}-S_K)_z]\}\ , \tag{4.1a}$$

$$(\ddot{S}_K)_z=8R^2\{(S_{K+1}+S_{K-1}-2S_K)_z+\tfrac{3}{2}(1-R)[(S_{K+1}-S_K)_z^2-(S_{K-1}-S_K)_z^2] +\tfrac{1}{4}(1-3R)[(S_{K+1}-S_K)_y^2-(S_{K-1}-S_K)_y^2]\}\ . \tag{4.1b}$$

In Eqs. (4.1) the subscripts y and z denote the components of the displacement in the y and z directions, respectively, and R is a dimensionless parameter representing the degree of nonlinearity in the Morse potential. Before proceeding to the expansion we note that Eq. (4.1) has been spatially normalized with respect to the cube edge of the cell a_0. Define ($\partial_K \leftrightarrow \partial_z$)

$$U \equiv \frac{\partial (S_K)_y}{\partial z}, \quad V \equiv \frac{\partial (S_K)_z}{\partial z} \tag{4.2}$$

to obtain

$$\begin{aligned} \frac{\partial^2 U}{\partial t^2} &= \frac{\partial^2}{\partial z^2}(U + 2b_0 UV) + \frac{1}{12}\frac{\partial^4 U}{\partial z^2 \partial t^2}, \\ \frac{\partial^2 V}{\partial t^2} &= \frac{\partial^2}{\partial z^2}(2V + b_1 V^2 + b_0 U^2) + \frac{1}{12}\frac{\partial^4 V}{\partial z^2 \partial t^2}. \end{aligned} \tag{4.3}$$

Here t is a dimensionless time normalized by $2R(m/D)^{1/2}a_0$, where m is the atomic mass and D is the dissociation energy of a single, isolated atom pair and

$$b_0 = (1-3R)/2, \quad b_1 = 3(1-R). \tag{4.4}$$

In terms of the original displacements $\phi \equiv S_y$ and $\psi \equiv S_z$ (with the index K dropped) Eq. (4.3) is derivable from Lagrangian density (here the index letter refers to partial differentiation)

$$\begin{aligned} \mathcal{L} = {} & \tfrac{1}{2}[(\phi_t)^2 + (\psi_t)^2] \\ & - \left[\frac{1}{2}(\phi_z)^2 + (\psi_z)^2 + b_0(\phi_z)^2 \psi_z + \frac{b_1}{3}(\psi_z)^3 \right] \\ & + \tfrac{1}{24}[(\phi_{zt})^2 + (\psi_{zt})^2], \end{aligned} \tag{4.5}$$

which, as expected, reveals the existence of an energy integral. A number of other conservation laws are also available.

In passing we note that, while at a first glance it seems that as far as traveling waves are concerned both the unregularized and regularized Eq. (4.3) are equivalent, there is a subtle difference between the two systems. This has to do with the very different way that the width of the solitary wave scales with its amplitude. While the width of the solitary wave which originates from the nonregularized equations (exactly like in the KdV case) is inversely proportional to its amplitude, in the present theory the width of a large-amplitude solitary wave appears to be independent of its amplitude. Further study of Eqs. (4.3) is on its way and will be reported in a future publication.

V. SUMMARY

This paper was concerned with the problem of how to describe the dynamics of a dense lattice. Differently stated, our aim was to exploit the proximity to continuum while preserving the essential features of the discrete system. This close-to-infinity domain is exactly the opposite domain of the few-particle lattice studied by means of dynamical systems techniques.

The idea of how to regularize the expansion around the discrete parameter l as outlined in the Introduction was then applied to more-complex configurations, each of which necessitates the use of a variation on the original theme. Each of the new evolution equations derived will have to be studied separately. From the point of view of analysis each of these equations is a convenient vehicle to study the dynamics of a dense lattice. This is to be contrasted with the ill-posed equations derived in previous work by using the direct expansion. The only use made of these ill-posed equations (apart of the singular case of the quadratic Boussinesq equation which is exactly integrable[11]) was to calculate a solitary wave.

We also mention here the Frankel-Kontorova problem in two dimensions. If nonharmonic interparticle forces are included, instead of the Sine-Gordon equation, one derives Eq. (3.22) in which dispersion plays a crucial role in arresting the formation of shock waves into which the system is propelled by the nonharmonic forces.

The method used in this work could further be applied to study (a) more-complex multidimensional lattices and (b) semiclassical systems which have a coherent state (e.g., Ref. 12 which deals with magnetic chains). In both classes of problems the behavior of a dense system is of great interest and importance.

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*Permanent address.

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