## Brief Reports

*Brief Reports are short papers which report on completed research which, while meeting the usual* **Physical Review** *standards of scientific quality, does not warrant a regular article. (Addenda to papers previously published in the* **Physical Review** *by the same authors are included in Brief Reports.) A Brief Report may be no longer than 3½ printed pages and must be accompanied by an abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

# Channeling continuum model derivation by method of averaging

T. J. Burns
*Sandia National Laboratories, Albuquerque, New Mexico 87185*

J. A. Ellison
*University of New Mexico, Albuquerque, New Mexico 87131*
(Received 13 June 1983)

Derivations of the axial- and planar-channeling continuum models from the perfect-string and perfect-plane models by the Krylov-Bogoliubov method of averaging are discussed. For the first time, error bounds are obtained relating the perfect crystal trajectories to the continuum-model trajectories. Details are presented for the axial case, because this case is easier to treat and the generalization to planes is straightforward.

A commonly used approximation in particle channeling calculations is called the continuum model.[1] In this model, the strings or planes of atoms of a perfect crystal are replaced by continuum strings or planes. Continuum ideas were discussed early by Lehmann and Leibfried,[2] Lindhard,[3] and Nelson and Thompson.[4] The validity of the continuum-string model, as an approximation to the perfect-string model, has been discussed[3–7] by comparing it with the impulse-momentum approximation to the perfect-string model. It is typically argued that the continuum model is a good approximation if a certain combination of physical parameters is small. However, no explicit error bounds on trajectories have been obtained, although Lindhard[3] has shown that the trajectories in the impulse-momentum approximation approximately conserve transverse energy. Because the impulse-momentum argument does not work in the case of planes, the relationship between the planar-continuum model and the associated perfect-plane model has not been adequately assessed.

In this paper, the relation between the solutions of the continuum-model equations of motion and the corresponding solutions of the perfect crystal equations are discussed. Error bounds relating trajectories of the two models, in the string case, are obtained under the assumption that the perfect-string trajectory has a positive minimum distance $\delta$ of approach to the string. The technique for finding the bounds can be generalized to planes and this is briefly discussed. An important complementary problem, which is of particular importance in the planar case, is to characterize those perfect-crystal trajectories that have a positive minimum distance of approach to strings or planes. Some promising work in this direction is being done by Saénz[8] and Nagel.

A standard approach to difficult problems in classical mechanics is to transform the differential equations into a set of equivalent equations with simpler structure. In the present context, the ideal would be to find an explicit transformation which transforms the perfect-crystal equations into the continuum-model equations, but this is probably not possible. Here, a transformation is presented which transforms the perfect-crystal equations into the continuum equations with higher-order corrections. The transformation is found by the method of averaging of Krylov and Bogoliubov.[9] This method has three important features: (1) The averaging transformation essentially averages out the lattice periodicities by putting them into the higher-order terms of the transformed equations, and the continuum model is obtained by neglecting these higher-order terms. (2) Knowledge of this transformation and the solutions of the continuum equations allows short-term periodicities to be put back in, thus improving on the continuum approximation. (3) Bounds on the errors are easily obtained under the *a priori* assumption that a particle in the perfect-crystal model does not approach a string or plane too closely.

Consider a charged particle with speed $v$ moving at an angle $\psi$ with respect to an infinite string of atoms of spacing $d$ along the $z$ axis, as illustrated in Fig. 1. The equations of motion are

$$m\frac{d^2x}{dt^2}=-\frac{\partial V}{\partial x},\quad m\frac{d^2z}{dt^2}=-\frac{\partial V}{\partial z}\quad, \tag{1}$$

and the associated energy is

$$\tfrac{1}{2}m(\dot{x}^2+\dot{z}^2)+V(x,z)=E\quad. \tag{2}$$

Here, $V(x,z)$ is the sum of the particle-atom potentials

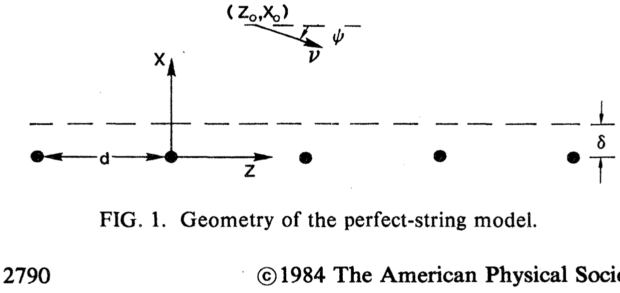


FIG. 1. Geometry of the perfect-string model.

$V(r)=Z_1Z_2e^2\phi(r/a)/r$ over all atoms in the string, where $Z_1$ and $Z_2$ are the atomic numbers of the projectile and lattice atoms, respectively, $e$ is the electronic charge, $a$ is the Thomas-Fermi screening radius, and $\phi$ is a screening function. For the infinite string $V$ is periodic in $z$, i.e., $V(x,z+d)=V(x,z)$. Only those trajectories with initial conditions $(x,\dot{x},z,\dot{z})=(x_0,\ -v\sin\psi,\ z_0,\ v\cos\psi)$ such that

$$\min_{t\geq 0} x(t)=\tilde{\delta}>0 \tag{3}$$

will be considered here.

Under channeling conditions, it is expected that $\psi$ is small, that $\frac{1}{2}m\dot{z}^2\simeq\frac{1}{2}m(v\cos\psi)^2\simeq E$ and that the energies $\frac{1}{2}m\dot{x}^2$ and $V(x,z)$ are roughly the same size. Let $K=2Z_1Z_2e^2/d$, which is related to the size of the potential. Then the above suggests introducing the dimensionless quantities

$$\begin{aligned} &X=x/d,\quad Z=z/d,\quad W(X,Z)=V(x,z)/K\ ,\\ &\Psi=\dot{x}/(2K/m)^{1/2},\quad \Phi=\dot{z}/(v\cos\psi),\quad \tau=(v\cos\psi/d)t\ . \end{aligned} \tag{4}$$

Note that $\psi$ cannot equal $\pi/2$ and that, for $\dot{z}$ constant, $\tau$ changes by one unit as the particle travels one lattice spacing. If Eqs. (1) are written as a first-order system, then the nondimensionalization (4) leads to

$$\begin{aligned} &\frac{dX}{d\tau}=\psi_1\Psi,\quad X(0)=X_0,\\ &\frac{d\Psi}{d\tau}=-\tfrac{1}{2}\psi_1\frac{\partial W(X,Z)}{\partial X},\quad \Psi(0)=-\frac{\tan\psi}{\psi_1}\equiv\Psi_0\ ,\\ &\frac{d\Phi}{d\tau}=-\tfrac{1}{2}\psi_1^2\frac{\partial W(X,Z)}{\partial Z},\quad \Phi(0)=1\ ,\\ &\frac{dZ}{d\tau}=\Phi,\quad Z(0)=Z_0\ , \end{aligned} \tag{5}$$

where the perturbation parameter

$$\psi_1=\{2Z_1Z_2e^2/[(md/2)(v\cos\psi)^2]\}^{1/2}$$

is equal to $(2Z_1Z_2e^2/dE)^{1/2}$ for small $\psi$. This is the angle introduced by Lindhard,[3] and it contains the main parameter dependencies of the channeling critical angle, namely, energy, atomic number, and lattice spacing. The perfect-string equations (5) have a periodic right-hand side with period 1 and are now written in a standard form for the method of averaging.[10] There is an unusual feature of (5) in that the perturbation parameter enters the initial data in a singular way. However, this is easily understood, since it is expected that $\psi=O(\psi_1)$. For bounded $W$ derivatives and $\psi_1$ small, $X$, $\Psi$, and $\Phi$ are slow variables, i.e., slowly varying with $\tau$, and $Z$ is a fast variable.

The associated equations for the continuum-string model are given by the averaged equations

$$\begin{aligned} &\frac{dX^*}{d\tau}=\psi_1\Psi^*\ ,\quad \frac{d\Psi^*}{d\tau}=-\tfrac{1}{2}\psi_1\overline{W}'(X^*)\ ,\\ &\frac{d\Phi^*}{d\tau}=0\ ,\quad \frac{dZ^*}{d\tau}=\Phi^*\ , \end{aligned} \tag{6}$$

where the starred variables denote approximations to the corresponding unstarred variables in (5). The approximate equations (6) are obtained by the method of averaging, as discussed below. In (6),

$$\overline{W}(X)=\int_0^1 W(X,Z)\,dZ \tag{7}$$

is a normalized continuum potential, and $\overline{W}'(X)$ approaches infinity as $X$ approaches zero for screening functions $\phi$ of channeling interest. Thus there is an obvious qualitative difference in the properties of certain solutions of Eqs. (5) and (6); namely, some solutions of Eq. (5) can penetrate the string, but no solutions of Eq. (6) can do this. This further points out the need for the *a priori* bound (3) in order for (6) to be a good approximation to (5). Notice that since $\Phi(0)=1$, Eq. (6) reduces to

$$\frac{d^2X^*}{dZ^{*2}}+\tfrac{1}{2}\psi_1^2\overline{W}'(X^*)=0\ . \tag{8}$$

In Lindhard's derivation[3] of the channeling critical angle $\psi_c$, he assumed the validity of the continuum model (6) and then showed that $\psi\leq\psi_c$ if, and only if, a continuum-model trajectory passes at least two lattice atoms in a collision with a continuum string. Here $\psi_c$ is defined implicitly by the unique solution of $E\psi_c^2=U(\psi_c d)$, where $U=K\overline{W}$ is the continuum potential for a string. He then showed, using the standard potential, that for large energies, the solution of this equation is approximately given by $\psi_c=c\psi_1$, where $\psi_1$ is the above perturbation parameter and $1\lesssim c\lesssim 3$. This quantity has turned out to be a basic experimental parameter for axial channneling and characterizes, for example, wide-angle scattering through several orders of magnitude in the incident energy.

The basic idea involved in using the Krylov-Bogoliubov method of averaging[10] to derive the continuum approximation (6) from the perfect-string model (5) is the following. Since the rate of change of the slow variable $\Psi$ depends on $Z$ in a periodic manner, intuition suggests that, over a long interval in the scaled time $\tau$, the $Z$ average over one period of $\partial W/\partial X$ with the slow variable $X$ held fixed, should determine most of the long-term change in $\Psi$, while the effect of the small oscillations about the average should be less important. Explicitly, the method of averaging can be used to construct a transformation of variables of the form

$$\begin{aligned} &X=u_1\ ,\quad \Psi=u_2+\psi_1P(u_1,u_3,w)\ ,\\ &\Phi=u_3,\quad Z=w\ , \end{aligned} \tag{9}$$

which transforms the perfect-crystal equations (5) into the simpler system

$$\begin{aligned} &\frac{du_1}{d\tau}=\psi_1u_2+\psi_1^2P, && u_1(0)=X_0\ ,\\ &\frac{du_2}{d\tau}=-\tfrac{1}{2}\psi_1\overline{W}'(u_1)+\psi_1^2G, && u_2(0)=\Psi_0-\psi_1P(X_0,1,Z_0)\ ,\\ &\frac{du_3}{d\tau}=-\tfrac{1}{2}\psi_1^2\frac{\partial W(u_1,w)}{\partial w}, && u_3(0)=1\ ,\\ &\frac{dw}{d\tau}=u_3, && w(0)=Z_0\ , \end{aligned} \tag{10}$$

with

$$G=-u_2P_{u_1}-\psi_1PP_{u_1}+\tfrac{1}{2}P_{u_3}W_w\ .$$

These are clearly perturbed continuum equations, and if the $O(\psi_1^2)$ terms are small, the solutions of (10) should be in good agreement with solutions of the continuum equations (6).

Under the *a priori* assumption (3), $u_1\geq\delta>0$, where $\delta=\tilde{\delta}/d$, and for this range of $u_1$, $P$ is a bounded function which is uniquely defined by the equation

$$\frac{\partial P}{\partial w}=-\frac{1}{2u_3}\frac{\partial}{\partial u_1}[W(u_1,w)-\overline{W}(u_1)] \tag{11}$$

and the conditions that $P$ be periodic in $w$ of period 1 with zero mean. Two infinite series representations for $P$ have been derived and are being analyzed. Also, for $u_1 \geqslant \delta > 0$, the function $G$ in Eq. (10) is bounded. Therefore Eqs. (5) and (10) are equivalent for all $\psi_1$ and $X = u_1 \geqslant \delta > 0$.

The problem of finding the best possible error bounds is difficult, and a detailed discussion of error bounds will be presented elsewhere. Here a technique for obtaining crude bounds is briefly discussed. Subtraction of the continuum equations (6) from the perturbed continuum equations (10) yields

$$\frac{d(u_1 - X^*)}{d\tau} = \psi_1(u_2 - \Psi^*) + \psi_1^2 P \ ,$$
$$\frac{d(u_2 - \Psi^*)}{d\tau} = -\tfrac{1}{2}\psi_1[\overline{W}'(u_1) - \overline{W}'(X^*)] + \psi_1^2 G \ ,$$
$$\frac{d(u_3 - \Phi^*)}{d\tau} = -\tfrac{1}{2}\psi_1^2 \frac{\partial W}{\partial w} \ , \qquad (12)$$
$$\frac{d(w - Z^*)}{d\tau} = u_3 - \Phi^* \ .$$

For a given set of initial conditions, the *a priori* bound (3) assures that $u_1$ stays away from the string, and the infinite force in the continuum model keeps $X^*$ away. Let $\delta_{\min}$ denote the minimum distance of approach for $u_1$ and $X^*$; then for all $u_1$ and $X^* \geqslant \delta_{\min}$

$$|\overline{W}'(u_1) - \overline{W}'(X^*)| \leqslant \overline{W}''(\delta_{\min})|u_1 - X^*| \ ,$$

and there exist constants $g_1$, $g_2$, and $g_3$ such that $|P| \leqslant g_1$, $|G| \leqslant g_2$, and $|\partial W/\partial w| \leqslant g_3$. By integrating Eqs. (12) and using standard methods of differential equations (e.g., the Gronwall inequality) it is easy to obtain crude bounds on $|u_1 - X^*|$, $|u_2 - \Psi^*|$, $|u_3 - \Phi^*|$, and $|w - Z^*|$. It is interesting that these bounds can be shown to depend on $\psi_1^2 \overline{W}''(\delta_{\min})$, which is essentially the quantity $d^2U''/E$, where $U(x) = K\overline{W}(X)$, derived by Lindhard,[3] who has shown it plays a crucial role in establishing the validity of the continuum-string model at halfway planes. The transformation (9) can then be used to show that solutions of the perfect-string model (5) and the continuum model (6), with the initial conditions of Eq. (5), satisfy

$$|X - X^*| \leqslant C_1\psi_1, \quad |\Psi - \Psi^*| \leqslant C_2\psi_1 \qquad (13)$$

for all $\tau$, $0 \leqslant \tau \leqslant 1/\psi_1$, where $C_1$ and $C_2$ depend on $g_1$, $g_2$, $g_3$, and $\overline{W}''(\delta_{\min})$. Thus the continuum model gives a good approximation for trajectories which stay away from the strings when $\psi_1$ is small.

A better approximation to the solutions of Eq. (5) for all $\tau$, $0 \leqslant \tau \leqslant 1/\psi_1$, is obtained by solving the continuum equations (6) with the initial conditions of Eq. (10) and then approximating $X$ by $X^*$ and $\Psi$ by $\Psi^* + \psi_1 P(X^*, \Phi^*, Z^*)$. This has the effect of putting the short-term lattice periodicities, which have been averaged out, back into the approximation. The infinite series representations for $P$ are currently being studied so that practical use of this approximation can be made.

We have shown that the continuuum model emerges as the first term in a systematic perturbation procedure which also allows the computation of error bounds. We have considered particle motion with zero angular momentum with respect to a string, which is the least favorable case for the validity of the continuum model. The extension of our results to the case of nonzero angular momentum is trivial, which is not the case for the impulse-momentum procedure.

As mentioned in the introduction, the extension to planes is straightforward and has been discussed in a preliminary way in Ref. 11. The perfect-plane equations are similar to Eq. (5), except there are six equations rather than four. The averaging transformation is also similar to (9), but it is more difficult to determine an explicit representation for the function $P$, and the error bound calculations are similar but more complex. Details will be presented elsewhere.

The averaging-perturbation technique should be useful in a number of other channeling problems of which the following are exemplary. The axial to planar channeling transition problem[12,13] can be viewed in terms of "strings of strings," so that the method of averaging is a natural way to study this transition and the associated phenomenon of resonance dechanneling.[14] The continuum model has been used to study channeling in bent crystals,[15] and averaging may be helpful in studying the limitations of this assumption. The averaging technique provides a systematic way to incorporate lattice periodicities into the continuum model, and therefore it is an alternate way to study the effect of crystal lattice periodicity on channeling radiation.[16]


## ACKNOWLEDGMENTS

Conversations with E. Bonderup, W. T. Kyner, S. T. Picraux, and E. Uggerhøj are gratefully acknowledged. The work of T.J.B. was supported in part by the U.S. Department of Energy under Contract No. DE-AC04-76-DP00789. Sandia National Laboratories is a U.S. Department of Energy facility. The work of J.A.E. was supported in part by the National Science Foundation under Grant No. DMR-82-14301.



[1] D. S. Gemmell, Rev. Mod. Phys. 46, 129 (1974).
[2] C. Lehmann and A. Leibfried, J. Appl. Phys. 34, 2821 (1963).
[3] J. Lindhard, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 34, 14 (1965).
[4] R. S. Nelson and M. W. Thompson, Philos. Mag. 8, 1677 (1963).
[5] D. V. Morgan and D. Van Vliet, Radiat. Eff. 8, 51 (1971).
[6] M. W. Thompson, in *Channeling*, edited by D. V. Morgan (Wiley, New York, 1973).
[7] D. Van Vliet, in Ref. 6.
[8] A. W. Sáenz, Phys. Lett. 93A, 271 (1983).
[9] N. Krylov and N. N. Bogoliubov, Publ. Ukranian Acad. Sci. (Kiev) No. 8 (1934); N. N. Bogoliubov and Y. A. Mitropolsky, *Asymptotic Methods in the Theory of Nonlinear Oscillations* (Gordon and Breach, New York, 1961).
[10] V. I. Arnold, *Mathematical Methods of Classical Mechanics* (Springer-Verlag, New York, 1978), Sect. 52.
[11] J. A. Ellison, University of New Mexico Technical Report No. 300, 1974 (unpublished).
[12] G. Della Mea, A. V. Drigo, S. L. Russo, P. Mazzoldi, G. G. Bentini, A. Desalvo, and R. Rosa, Phys. Rev. B 7, 4029 (1973); A. Desalvo and R. Rosa, *ibid.* 9, 4605 (1974).
[13] S. D. Mukherjee and M. W. Thompson, Radiat. Eff. 55, 223 (1981); 56, 159 (1981).
[14] M. A. Kumakhov and R. Wedell, Phys. Status Solidi B 76, 119 (1976).
[15] J. A. Ellison, Nucl. Phys. B206, 205 (1982).
[16] G. Kurizki and J. K. McIver, Phys. Lett. 89A, 43 (1982).