

LEADING ORDER HARD EDGE FRINGE FIELDS EFFECTS EXACT IN $(1 + \delta)$ AND CONSISTENT WITH MAXWELL'S EQUATIONS FOR RECTILINEAR MAGNETS

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In a circular machine, where the linear lattice functions (α, β, γ) and a phase advance can be defined, one expects the fringe field effects to be negligible if the change in these functions is small through the element. However, this may not always be the case. In such situations, it is useful to have a leading order result which is adapted to tracking and analytical analysis. In this paper, we provide such a result for the quadrupole and we also provide a general formula for the effect of an arbitrary rectilinear multipole.

Starting from the standard multipole expansion for the \mathbf{B} field of a $2(n+1)$ -pole ($n \geq 1$), we compute the missing terms in the vector potential expansion consistent with the pure $2(n+1)$ -pole symmetry. We then compute the leading effects of the fringing fields of a multipole on the dynamics. Finally, we apply this result to quadrupoles and reproduce the original results of Lee-Whiting, Matsuda, and Wollnik.

For the quadrupole, we show how to write a symplectic (canonical) integrator for the dynamics which can be used in a standard circular machine kick code. For higher order multipoles, we display the implicit characteristic function solution as first proposed by Dragt.

1. Introduction

The field of beam optics is vast and diverse. The mathematical tools and the mathematical requirements of particle optics simulations are very different in small beam lines and in large circular machines.

One unfortunate result of this diversity is reflected in the lack of cross-referencing between the fields of electron-microscopy and ion spectroscopy on the one hand, and large circular machine optics on the other. An even more unfortunate aspect of this alienation is a mutual ignorance of each other's techniques and methods. In an effort to remedy this situation two international beam optics conferences have been organized, the first one at Giessen [1] (FRG) and the second one at Albuquerque [2] (NM, USA). In this paper we will attempt to solve completely a simple problem, blending in the tools of beam optics (Lie operator methods and characteristic functions) with the concerns of large circular machine theorists ("symplecticity" and exact energy-dependence). First, let us contrast these two extreme fields of particle tracking. What follows may sound like an exaggeration, but is close enough to the truth to have generated two international conferences.

Typically in ion optics [3] one is interested in gaining a precise knowledge of the optics of a relatively small set of electric and magnetic elements. As a result, a considerable effort has been put into the derivation of linear and nonlinear transport matrices for various beam elements.

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In particular, many authors have looked seriously at the effect of fringe fields on the transfer matrices. In particular, Lee-Whiting [4] has shown that the effect of a quadrupole entrance fringe field is given to first order by:

$$\Delta x = \left(\frac{1}{12}x^3 + \frac{1}{4}xy^2 \right) k_0, \tag{1a}$$

$$\Delta p_x = \left[\frac{1}{2}xyp_y - \frac{1}{4}p_x(x^2 + y^2) \right] k_0, \tag{1b}$$

$$k_0 = \frac{B'}{B\rho} \text{ at the center of the magnet.} \tag{1c}$$

Needless to say, opticians interested in spectroscopy did not confine themselves to first order results. Lee-Whiting, and later Matsuda and Wollnik [5], have derived corrections to eq. (1) which depend on the higher derivatives in z of the field gradient B' .

This attention to details has to be contrasted to the field of high energy circular machines where Maxwellian fringe field effects are neglected, with the notable exception of the vertical focussing of a bend, which is Maxwellian. Moreover, it is customary in the study of large circular machines to use models in which the dipoles and quadrupoles are simple linear maps. This will seem to be a heresy to the reader accustomed to ion spectroscopy and electron microscopy. Conversely, the spectroscopist's attention to field details is often surprising to people designing large machines.

Another issue which distinguishes circular machines from small single pass systems is "symplecticity". In ion spectrometers, the tracking procedure provided by nonlinear matrix codes need not satisfy Liouville's theorem. In fact, in general, if the Taylor series expansion used in these codes is accurate to some degree k , Liouville's theorem will be satisfied to the same degree k . This can become a problem if a map is to be iterated a large number of times, as is done in the study of circular machines, because a spurious growth of phase space may result from a small violation of the symplectic conditions [6].

Circular machine scientists have unconsciously solved this problem by using linear maps and multipole kicks in their tracking programs. These elements produce automatically symplectic maps. In fact, these methods are under the more general topic of symplectic integration. Finally, it can be said that one can "symplectify" a Taylor series code using Lie operators as shown by Dragt in his code MARYLIE [7]. Because one can compute a Lie polynomial representation from a nonlinear matrix, it is also true that one may produce symplectic tracking with a standard matrix code.

In this paper, we will generalize the result of Lee-Whiting to a rectilinear multipole of arbitrary degree. In the spirit of large machine physicists, we will keep the δ -dependence ($\delta = (p - p_0)/p_0$) of the map exact. We will derive our results using the powerful tools of Lie operators and Hamiltonian mechanics [8]. For the case of the quadrupole, we will provide an explicit symplectic formula for eq. (1) which includes the effects on the time of flight. For the other multipoles, a symplectic tracking procedure can easily be derived using the Lie operator and a first order equivalent characteristic function.

Purposely, this paper looks at a simple unsolved problem from a very wide angle. As a result, we will probably disturb the ion spectrometer specialist, as well as the large machine optician, by our use of a large spectrum of techniques. But we believe that the accelerator-spectrometer-microscopy theorists and designers would benefit from a greater exposure to all the various techniques of beam optics.

Finally, the reader will notice that we neglected the case of bending magnets. Bending magnets are more subtle. However, from the point of view of the spectrometer scientists, nothing needs to be added. On the other hand, a lot of misconceptions inundate the field of large machine physics. This topic is covered in a Superconducting Super Collider (SSC) technical report [9].

2. Derivation of a potential $\Phi_{n+1}(r, \phi, z)$ for a z -dependent $2(n+1)$ -pole

In this paper, we found it easy to work directly with the Hamiltonian and the formulae connecting H with the Lie generators of the motion through the fringing fields. This allows for a simpler treatment and

understanding of all the discontinuities which arise in the hard edge limit. For example, it will be clear from our treatment that if the leading effect of the body of a $2(n+1)$ -pole is of order n , a finite fringe field effect occurs at the order $n+2$.

For a Hamiltonian treatment, we must derive an expansion of the vector potential which is based on the axial field gradients and obeys Maxwell's equations. To get this vector potential, it is convenient to rederive a famous formula for the scalar potential $\Phi(\mathbf{B} = \nabla\Phi)$ [10].

Consider a field represented by the expansion:

$$B_y + iB_x = B_0 \sum_{n=1}^{\infty} (ia_n + b_n)(x + iy)^n \quad (2)$$

We can write a vector potential for this field:

$$A_z = -\text{Re} \left[B_0 \sum_{n=1}^{\infty} \frac{1}{n+1} (ia_n + b_n)(x + iy)^{n+1} \right]. \quad (3)$$

Let us rewrite eq. (2) in polar coordinates:

$$B_y + iB_x = B_0 \sum_{n=1}^{\infty} C_n r^n e^{in\phi}, \quad (4a)$$

$$x = r \cos \phi, \quad (4b)$$

$$y = r \sin \phi, \quad (4b)$$

$$C_n = ia_n + b_n. \quad (5)$$

If B_0 is some function of z , the longitudinal variable, Maxwell's equation is violated. We will derive the corrections on \mathbf{B} needed to satisfy Maxwell's equations.

Assuming that $\mathbf{B} = \text{Re} \nabla\Phi$, then the following must be true in a current free region:

$$\nabla^2 \Phi = 0. \quad (6)$$

Furthermore, since $[\nabla^2, \partial/\partial\phi]$ vanishes, we can diagonalize ∇^2 and $\partial/\partial\phi$ simultaneously. In other words, we can look at an individual multipole alone.

Assume that $\Phi_{n+1}(r, \phi, z)$ has the form:

$$\Phi_{n+1} = e^{i(n+1)\phi} \psi_{n+1}(r, z) = \left(\sum_{m=0}^{\infty} A_m(z) r^m \right) e^{i(n+1)\phi}. \quad (7)$$

Then, according to Laplace's equations in cylindrical coordinates, we must have:

$$\sum_{m=1}^{\infty} A_{m+2} (m+2)^2 r^m + \sum_{m=0}^{\infty} A_m'' r^m - \frac{(n+1)^2}{r^2} \psi_{n+1} = 0, \quad (8a)$$

or,

$$\sum_{m=0}^{\infty} \left[(m+2)^2 A_{m+2} + A_m'' - (n+1)^2 A_{m+2} \right] r^m + \frac{A_1}{r} - \frac{(n+1)^2}{r} A_1 - \frac{(n+1)^2}{r^2} A_0 = 0. \quad (8b)$$

Here the primes indicate a derivative with respect to z . We get from eq. (8b) a recursion formula for the A_m 's.

$$A_{m+2} = \frac{A_m''}{(n+1)^2 - (m+2)^2} = \frac{-A_m''}{(m+n+3)(m+1-n)}. \quad (9)$$

If we correctly assume that A_{n+1} is the first nonzero coefficient, we get for ψ_{n+1} :

$$\psi_{n+1}(r, z) = \sum_{l=0}^{\infty} \frac{A_{n+1}^{[2l]} (-1)^l (n+1)! r^{2l+n+1}}{2^{2l} l! (l+n+1)!}; \quad n \geq 1. \tag{10a}$$

$$A_{n+1}^{[2l]} = (2l)\text{th derivative in } z. \tag{10b}$$

Consider the r^{n+1} terms in eq. (4a), and match them to eq. (2):

$$i(n+1)A_{n+1} = B_0 C_n, \quad A_{n+1} = \frac{-i B_0 C_n}{n+1}. \tag{11}$$

Hence, we get for $\psi_{n+1}(r, z)$:

$$\psi_{n+1}(r, z) = \frac{-i C_n}{n+1} \sum_{l=0}^{\infty} (-1)^l \frac{B_0^{[2l]} (n+1)!}{2^{2l} l! (l+n+1)!} r^{2l+n+1}; \quad n \geq 1. \tag{12}$$

3. Derivation of a proper vector potential

For $n \geq 1$ (quadrupole and higher), we will assume that only the A_r and A_z components are needed. We must have:

$$B_z = -\frac{1}{r} \frac{\partial}{\partial \phi} A_r^{n+1} = \frac{\partial}{\partial z} \Phi_{n+1}, \tag{13a}$$

$$B_r = \frac{1}{r} \frac{\partial}{\partial \phi} A_z^{n+1} = \frac{\partial}{\partial r} \Phi_{n+1}, \tag{13b}$$

$$B_\phi = \frac{\partial A_r^{n+1}}{\partial z} - \frac{\partial A_z^{n+1}}{\partial r} = \frac{1}{r} \frac{\partial}{\partial \phi} \Phi_{n+1}. \tag{13c}$$

It is easy to check that A_r^{n+1} and A_z^{n+1} are given by:

$$A_r^{n+1} = \frac{ir}{n+1} \frac{\partial \psi_{n+1}}{\partial z} e^{i(n+1)\phi}, \tag{14a}$$

$$A_z^{n+1} = \frac{-ir}{n+1} \frac{\partial \psi_{n+1}}{\partial r} e^{i(n+1)\phi}. \tag{14b}$$

Indeed eqs. (13a) and (13b) are automatically satisfied by eqs. (14), and eq. (13c) follows from Laplace's equation. From now on, one must always remember that the real part of \mathcal{A} must be put into the Hamiltonian.

4. Computation of the fringe field effects in the limit of a hard edge

For a rectilinear system, we can write the Hamiltonian as follows [11].:

$$H = -\sqrt{(1+\delta)^2 - (p_x - \tilde{A}_x)^2 - (p_y - \tilde{A}_y)^2} - \tilde{A}_z - p_r/\beta, \tag{15}$$

where \tilde{A}_i is just:

$$\tilde{A}_i = \frac{q}{p_0} A_i = \frac{1}{B\rho} A_i. \tag{16}$$

Here (x, y) are the usual transverse variables and (p_x, p_y) are the momenta scaled by p_0 . The pair τ and p_r are the differential time $c(T - T_0)$, and the differential energy $(E_0 - E)/p_0c$, respectively. The quantity β is the design velocity over the speed of light.

At the entrance of a magnet, the function $B_0(z)$ has the form:

$$B_0(z) \equiv \hat{B}\theta(z), \quad (17)$$

where $\theta(z)$ is the usual unit step function, and \hat{B} is the constant mid-magnet strength of $B_0(z)$. Let us expand A_r^{n+1} and A_z^{n+1} beyond their usual ideal expansion using eq. (14):

$$\psi_{n+1} = \frac{-i\hat{B}C_n}{n+1} \left(\theta r^{n+1} - \frac{\theta'' r^{n+3}}{4(n+2)} + \dots \right), \quad (18a)$$

$$A_r^{n+1} = \frac{\hat{B}C_n \theta' r^{n+2}}{(n+1)^2} e^{i(n+1)\phi} + \dots, \quad (18b)$$

$$A_z^{n+1} = \frac{-C_n \hat{B}}{(n+1)^2} \left[\theta(n+1)r^{n+1} - \frac{\theta''(n+3)}{4(n+2)} r^{n+3} + \dots \right] e^{i(n+1)\phi}. \quad (18c)$$

We notice that in the Hamiltonian H , the correction introduced by Maxwell's equations is of degree $n+3$, while the original multipole is of degree $n+1$. In fact, let us expand H in powers of r and p to order $n+3$;

$$H \approx \frac{p_x^2 + p_y^2}{2(1+\delta)} - \frac{\tilde{A}^{n+1}}{1+\delta} \cdot p - \tilde{A}_{n+1}^z + \dots, \quad (19a)$$

$$H \approx \frac{p_r^2}{2(1+\delta)} + \frac{p_\phi^2}{2(1+\delta)r^2} + \left[\frac{\tilde{C}_n \hat{B}}{n+1} \theta r^{n+1} - \frac{\tilde{C}_n \hat{B}(n+3)}{(n+1)^2 4(n+2)} \theta'' r^{n+3} - \frac{\tilde{C}_n \hat{B} \theta'}{(1+\delta)(n+1)^2} r^{n+2} p_r \right] \exp(i(n+1)\phi), \quad (19b)$$

$$\tilde{C}_n = \frac{qC_n}{p_0} = \frac{q}{p_0} (ia_n + b_n), \quad (19c)$$

$$rp_r = xp_x + yp_y, \quad (19d)$$

$$p_\phi = xp_y - yp_x. \quad (19e)$$

In the hard edge limit θ' and θ'' become the Dirac delta function and its derivative. We must handle the computation with care. We split the Hamiltonian H of eq. (19b) in three parts:

$$H = D + \theta V_0 + \theta' V_1 + \theta'' V_2 \quad (20a)$$

$$= D + V. \quad (20b)$$

Let us solve for the map $\mathcal{M}(\epsilon)$, which brings the particle between $-\epsilon$ and ϵ in the limit of ϵ going to zero and to first order in V . According to a standard result of map theory [7]:

$$\mathcal{M}(\epsilon) = \exp(:f:) \exp(:-2\epsilon D:) + O(V^2), \quad (21a)$$

$$\mathcal{D}(z) = \exp(:-(z+\epsilon)D:), \quad (21b)$$

$$f = - \int_{-\epsilon}^{\epsilon} \mathcal{D}(z) V dz, \quad (21c)$$

$$:f:g = [f, g] \equiv \text{Poisson bracket}. \quad (21d)$$

In the limit of ϵ going to zero, \mathcal{D} becomes the identity map, and the terms in θ and θ' can be evaluated immediately:

$$f_0 = \lim_{\epsilon \rightarrow 0} \left(- \int_{-\epsilon}^{\epsilon} \mathcal{D}(z) \theta V_0 dz \right) = 0, \tag{22a}$$

$$f_1 = \lim_{\epsilon \rightarrow 0} \left(- \int_{-\epsilon}^{\epsilon} \mathcal{D}(z) \theta' V_1 dz \right) = -V_1. \tag{22b}$$

For the term in θ'' , we integrate by parts:

$$f_2(\epsilon) = - \int_{-\epsilon}^{\epsilon} \mathcal{D}(z) \theta'' V_2 dz = - \mathcal{D}(z) \theta' V_2 \Big|_{-\epsilon}^{\epsilon} + \int_{-\epsilon}^{\epsilon} \left[\frac{d}{dz} \mathcal{D}(z) \right] \theta' V_2 dz,$$

$$\lim_{\epsilon \rightarrow 0} f_2(\epsilon) = \lim_{\epsilon \rightarrow 0} \frac{d}{dz} \mathcal{D}(z) V_2 \Big|_{z=0} = \lim_{\epsilon \rightarrow 0} \mathcal{D}(z) : -D : V_2 \Big|_{z=0} = [V_2, D]. \tag{23}$$

The final map is just:

$$\mathcal{M} = \exp (:f:), \tag{24a}$$

$$f = \text{Re}(-V_1 + [V_2, D]), \tag{24b}$$

$$V_1 = - \exp(i(n+1)\phi) \frac{\tilde{C}_n \hat{B}}{(1+\delta)(n+1)^2} p_r r^{n+2}, \tag{24c}$$

$$V_2 = - \exp(i(n+1)\phi) \frac{\tilde{C}_n \hat{B}(n+3)}{(n+1)^2 4(n+2)} r^{n+3}, \tag{24d}$$

$$D = \frac{p_r^2 + p_\phi^2 / r^2}{2(1+\delta)}. \tag{24e}$$

We were allowed to ignore the “real part” until eqs. (24), since all calculations were linear in the multipole strength. Of course, for the exit face, one need only to switch the sign of f .

5. Application to quadrupoles

Consider the case of $n = 1$. Let us compute V_1 first,

$$V_1 = - \exp(i2\phi) \frac{\tilde{C}_1 \hat{B}}{(1+\delta)4} p_r r^3, \tag{25a}$$

and V_2 ,

$$V_2 = - \exp(i2\phi) \frac{\tilde{C}_1 \hat{B}}{12} r^4, \tag{25b}$$

$$[V_2, D] = \frac{\partial V_2}{\partial r} \frac{p_r}{1+\delta} + \frac{\partial V_2}{\partial \phi} \frac{p_\phi}{r^2(1+\delta)}$$

$$= - \exp(i2\phi) \frac{\tilde{C}_1 \hat{B}}{3} \frac{p_r r^3}{1+\delta} - i \exp(i2\phi) \frac{\tilde{C}_1 \hat{B}}{6(1+\delta)} r^2 p_\phi.$$

Finally, f is just:

$$f = \text{Re} \left[\exp(i2\phi) \frac{\tilde{C}_1 \hat{B}}{(1+\delta)} \left(- \frac{p_r r^3}{12} - i \frac{r^2 p_\phi}{6} \right) \right]. \tag{26}$$

We will discover that the expression for the skew quadrupole fringe field is simpler than its normal counterpart. Let us compute them using the expressions:

$$\frac{\tilde{C}_1 \hat{B}}{1 + \delta} = \frac{(i\tilde{a}_1 + \tilde{b}_1) \hat{B}}{1 + \delta}, \quad (27a)$$

$$rp_r = xp_x + yp_y, \quad (27b)$$

$$p_\phi = xp_y - yp_x. \quad (27c)$$

One gets for f :

$$f = \left(\frac{q\hat{B}}{p_0(1 + \delta)} \right) \left[b_1 \left(\frac{3x^2yp_y - 3y^2xp_x + y^3p_y - x^3p_x}{12} \right) + \frac{a_1}{6} (x^3p_y + y^3p_x) \right]. \quad (28)$$

The normal part of f in eq. (28) is not easy to evaluate to all orders because none of the terms are kicks. To first order, one regains out of f Lee–Whiting's expression (eq. (1)). However, the skew term is very simple to evaluate in a symplectic manner. We first factorize \mathcal{M} as follows:

$$\mathcal{M} = \exp(:f:) = \exp\left(:\alpha \frac{x^3p_y}{1 + \delta}:\right) \exp\left(:\alpha \frac{y^3p_x}{1 + \delta}:\right) + O(\alpha^2), \quad (29a)$$

$$\alpha = \frac{q\hat{B}a_1}{6p_0}. \quad (29b)$$

Notice that both factors in eq. (29a) are kicks! For example,

$$\exp\left(:\alpha \frac{y^3p_x}{1 + \delta}:\right) x = x - \frac{\alpha y^3}{1 + \delta}, \quad (30a)$$

$$\exp\left(:\alpha \frac{y^3p_x}{1 + \delta}:\right) p_y = p_y + \frac{3\alpha}{1 + \delta} y^2 p_x, \quad (30b)$$

$$\exp\left(:\alpha \frac{y^3p_x}{1 + \delta}:\right) \tau = \tau + \frac{\alpha y^3 p_x}{(1 + \delta)^2} \frac{d\delta}{dp_\tau}, \quad (30c)$$

where

$$1 + \delta = \sqrt{1 - \frac{2p_\tau}{\beta} + p_\tau^2}, \quad (30d)$$

$$\frac{d\delta}{dp_\tau} = \frac{p_\tau - 1/\beta}{1 + \delta}. \quad (30e)$$

Clearly the factor x^3p_y produces a map similar to eqs. (30) with x and y interchanged.

How do we represent a normal quadrupole fringe field using the result of eq. (30)? Obviously, we need only to rotate the skew quadrupole by $\pm 45^\circ$ to obtain the normal result.

In fact, one needs to rotate the beam by -45° , followed by the kick of eq. (30) and finally one “de”-rotates by 45° . With this prescription, a_1 is identified to b_1 . In other words, we have:

$$\alpha = \frac{q\hat{B}}{6p_0} a_1 \equiv \frac{1}{6B\rho} \frac{d\hat{B}_y}{dx} \equiv \frac{B'}{6B\rho} \equiv \frac{k_0}{6}. \quad (31)$$

6. Higher order multipoles

To get the higher order result, we apply eq. (25c) to the general expressions for V_2 . One gets the result:

$$f = -\text{Re} \left\{ \exp[i(n+1)\phi] \frac{\tilde{C}_n \hat{B}}{4(n+2)(1+\delta)} \left[r^{n+2} p_r + \frac{i(n+3)}{n+1} r^{n+1} p_\phi \right] \right\}, \tag{32a}$$

$$f = \frac{-\hat{B}}{4(n+2)(1+\delta)} \left[(cb_n - sa_n) r^{n+1} (xp_x + yp_y) - (sb_n + ca_n) \frac{n+3}{n+1} r^{n+1} (xp_y - yp_x) \right], \tag{32b}$$

where $c = \cos[(n+1)\phi]$ and $s = \sin[(n+1)\phi]$. (32c)

The expression (32b) for the polynomial f will not in general be a sum of kicks. In general they will look like the normal quadrupole term of eq. (28). It is possible, however, to transform f by a succession of linear transformations and turn the evaluation of $\exp(:f:)$ into a product of kicks. Unfortunately, the general theory for this has not been worked out. In fact, it will eventually involve a Clebsch–Gordan series for the symplectic group [12]. The minor miracle of the skew quadrupole does not happen for the fields above the quadrupoles.

Nevertheless, following a procedure used by Dragt [6] one can generate a symplectic map using the generating function F , defined by the relation

$$F = x\bar{p}_x + y\bar{p}_y + \tau\bar{p}_\tau - f(x, \bar{p}_x, y, \bar{p}_y, \bar{p}_\tau). \tag{33}$$

Using F we can generate a set of implicit equations which can be solved simply on the computer:

$$\begin{aligned} \bar{x} &= \frac{\partial F}{\partial \bar{p}_x}, & p_x &= \frac{\partial F}{\partial x}, \\ \bar{y} &= \frac{\partial F}{\partial \bar{p}_y}, & p_y &= \frac{\partial F}{\partial y}, \\ \bar{\tau} &= \frac{\partial F}{\partial \bar{p}_\tau}, & p_\tau &= \bar{p}_\tau. \end{aligned} \tag{34}$$

It is simple to check that the “bar” variables reproduce the action of $\exp(:f:)$ to first order in f .

In the absence of a general kick decomposition for f , eq. (34) is the only simple symplectic representation available. We hope that this will eventually change!

7. Conclusion

We can derive a symplectic representation of the first order fringe field of a quadrupole by realizing that a canonical integrator is easy to derive in the case of a skew quadrupole. The general quadrupole result is obtained by a rotation. (Similarity transformation.) This can be implemented easily in a large machine tracking code while preserving the canonical nature of the six-dimensional flow.

We also provided a general solution for arbitrary multipoles. Our Lie operator representation allows for a possible “symplectification” of the tracking procedure in which our formula may be used and therefore suits well the case of circular machines.

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This formula is often written with an extra $n!$ in the denominator.
- [11] A. Dragt and E. Forest, *Advances in Electronics and Electron Physics*, eq. (40) (1986) p. 77.
- [12] Private conversation with G. Rangarajan of the University of Maryland.