

## Concurrence in arbitrary dimensions

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(Received 7 August 2001; revision received 4 December 2001)

**Abstract.** We argue that a complete characterization of quantum correlations in bipartite systems of many dimensions may require a quantity which, even for pure states, does not reduce to a single number. Subsequently, we introduce multidimensional generalizations of concurrence and find evidence that they may provide useful tools for the analysis of quantum correlations in mixed bipartite states. We also introduce biconcurrence that leads to a necessary and sufficient condition for separability.

### 1. Introduction

Entanglement plays a central role in quantum information theory [1, 2]. Pure state entanglement of bipartite systems is well understood in the sense that the relevant parameters for its optimal manipulation by local operations and classical communication (LOCC) have been identified and analysed [2, 3]. Many efforts have also been devoted to the study of mixed-state entanglement. There, several possible entanglement measures have been proposed. Among these, entanglement ( $E_F$ ) of formation [4, 5] has attracted much attention, as it is closely connected with the rate of production of mixed bipartite states out of pure states by LOCC operations. It is, however, extremely difficult to evaluate  $E_F$ , with one exception: the analytical formula for  $E_F$  of a single copy of an arbitrary state of two qubits obtained by Wootters [6]. Despite efforts, there has not been much progress in generalizing Wootters' result to states in more than  $2 \times 2$  dimensions in [7],  $E_F$  for Woner states in arbitrary dimensions was obtained.

Wootters' success in quantifying  $E_F$  for two qubits can be attributed to associating  $E_F$  with concurrence which is easier to calculate than  $E_F$ . Concurrence, as introduced by Hill and Wootters [8], was defined via the operation of spin flip. More recently, Rungta *et al.* [9] made an attempt to generalize the notion of concurrence to pure bipartite states in arbitrary dimensions by introducing the

operation of universal state inversion. Similar operation has been independently considered in [10] in a different context. The universal inverter used by Rungta *et al.* generalizes spin flip to a transformation which brings a pure state  $|\psi\rangle$  into the maximally mixed state in the subspace orthogonal to  $|\psi\rangle$ . In the same way that the spin flip generates concurrence for a pair of qubits, the universal inverter generates a number which generalizes concurrence for joint pure states of pairs of quantum systems of arbitrary dimensions. Generalized in this way, concurrence measures entanglement of pure bipartite states in terms of the purity of their marginal density operators.

As is known [3], a complete characterization of quantum correlations in bipartite systems of many dimensions may require a quantity which, even for pure states, does not reduce to a single number. A single number is sufficient only for the *asymptotic* limit of many identical copies of bipartite pure states [11]. Take, for example, two pure states represented by vectors  $\psi = (|11\rangle + |22\rangle)/2$  and  $\phi = a\psi + b|33\rangle$ , with  $a = x^{1/2}$  and  $b = (1-x)^{1/2}$ , where  $x \approx 0.2271$  is a root of  $x^x[2(1-x)]^{1-x} = 1$ . The two states have the same entanglement  $E_F$  of 1 ebit; nevertheless they have different Schmidt numbers. Consequently, it is impossible to convert locally a finite number of copies of one state into the same number of copies of the other state.

In this contribution, we argue that a suitable generalization of spin flip to more dimensions should produce a multidimensional analogue of concurrence rather than a single number. Such a concurrence would then describe not only the *amount* of entanglement but also its *structure*, for example the size (the number of dimensions) of the entangled spaces on each side. Our concurrence for pure states is then associated with an operator transforming the exterior product of Alice's part of the bipartite Hilbert space with itself, that is  $H_A \wedge H_A$  into the exterior product of Bob's part of the bipartite Hilbert space with itself, that is  $H_B \wedge H_B$ .

Having defined concurrence for pure states, we follow Wootters and generalize the concept to mixed states by introducing a matrix of preconcurrence. The elements of this matrix are matrices in their own right and, at the end, our preconcurrence may be difficult to analyse. At least partially, the difficulty can be associated with the matrix dependence on the choice of the local bases. Therefore, we also generalize the concept of concurrence in a somewhat different direction. We abandon the requirement for preconcurrence to be a second-order object in the state's ensemble. For this price we can define a fourth-order object, a *biconcurrence* matrix. This matrix is independent of the local unitaries and allows us to reformulate the separability problem in terms of the matrix's main diagonal. Moreover, biconcurrence is a very simple function of the ensemble of the density matrix and has many symmetries. Consequently, the necessary and sufficient separability condition which follows from the structure of biconcurrence seems to be the most promising one from an algebraic point of view.

Our generalization of preconcurrence is presented in section 2. Then, in section 3 we give an example to show how our multidimensional preconcurrence can be used for the analysis of separability in arbitrary dimensions. There, we also discuss possible limitations of such analysis. Subsequently, in section 4 we introduce biconcurrence and formulate the necessary and sufficient condition for separability in terms of its elements. Finally, in section 5 we present a brief discussion of the results.

## 2. Spin flip and concurrence

### 2.1. Pure states

When acting in a two-dimensional vector space, a spin flip transforms a vector  $\mathbf{v}$  into another vector  $\tilde{\mathbf{v}}$  equally long and orthogonal to  $\mathbf{v}$ . In a bipartite system, a spin flip means that Alice performs a spin flip on her qubit and Bob on his. This gives a particularly simple expression for concurrence:

$$\mathbf{C}(\psi) = \langle \tilde{\psi} | \psi \rangle. \tag{1}$$

The spin-flip operation and the concurrence which follows are well defined since, in a two-dimensional space, there is only one direction which is orthogonal to a given direction. One may further note that concurrence defined in equation (1) together with the state's normalization allow us to determine the eigenvalues of the associated reduced density matrix and, via these, the pure state's entanglement. The eigenvalues are the squares of the singular values  $\lambda_1$  and  $\lambda_2$  of a  $2 \times 2$  matrix  $[\psi]$  of the coefficients defining the state in the standard basis:

$$|\psi\rangle = \sum_{i,j} \psi_{i,j} |i\rangle_A \otimes |j\rangle_B. \tag{2}$$

The singular values are then related to the concurrence via

$$|\mathbf{C}| = 2 \lambda_1 \lambda_2 = 2 |\det([\psi])|.$$

In general, in a  $d$ -dimensional space there are  $d - 1$  dimensions orthogonal to a given direction. These can be represented by a  $d - 1$  antisymmetric form. From this point of view, performing a spin flip on a bipartite state means constructing a double  $d - 1$  form (one side for Alice and one side for Bob) locally dual to the double one-form representing the state vector  $|\psi\rangle$ . Concurrence can then be associated with the contraction of the form representing  $|\psi\rangle$  with the form representing  $\langle \tilde{\psi} |$ . The contraction gives a double  $(d - 2)$ -form which is equivalent to a double two-form and can be represented by a  $\binom{d}{2} \times \binom{d}{2}$  matrix with the following elements:

$$C_{i_1 \wedge j_1; i_2 \wedge j_2} = 2(\psi_{i_1, i_2} \psi_{j_1, j_2} - \psi_{i_1, j_2} \psi_{j_1, i_2}). \tag{3}$$

These elements are easily identified as twice the two-dimensional minors of matrix  $[\psi]$ . They describe the two-state contributions to the bipartite entanglement.

Regarding their structure, matrices  $\mathbf{C}$  form a vector space with a natural trace norm:

$$|\mathbf{C}|^2 = \text{Tr}(\mathbf{C}\mathbf{C}^\dagger) = \sum_{i \wedge j, k \wedge l} |C_{i \wedge j; k \wedge l}|^2. \tag{4}$$

Having constructed the concurrence matrix, one may proceed in the same spirit and construct higher-dimensional minors of  $[\psi]$  (up to the Schmidt number). They will represent those contributions to the bipartite entanglement which embrace local subspaces of higher dimensions. We believe that, in principle, these concurrences of order higher than two may be important for the quantification of entanglement even if the separability of a pure state is determined by the lowest-order (i.e. two) concurrence. Clearly, a pure state (2) in arbitrary dimensions is separable if  $[\mathbf{C}] = 0$ .

2.2. *Mixed states*

In order to generalize further the concept of concurrence to multidimensional mixed states, we follow Wootters and introduce preconcurrence as follows. Given a decomposition of state  $\varrho$  into pure unnormalized states, that is

$$\varrho = \sum_{\mu} |\psi^{\mu}\rangle\langle\psi^{\mu}|, \tag{5}$$

we define preconcurrences

$$\begin{aligned} C_{i_1 \wedge j_1; i_2 \wedge j_2}^{\mu\nu} &= \psi_{i_1, i_2}^{\mu} \psi_{j_1, j_2}^{\nu} - \psi_{i_1, j_2}^{\mu} \psi_{j_1, i_2}^{\nu} \\ &\quad + \psi_{i_1, i_2}^{\nu} \psi_{j_1, j_2}^{\mu} - \psi_{i_1, j_2}^{\nu} \psi_{j_1, i_2}^{\mu} \end{aligned}$$

The preconcurrences can be regarded as a set of  $\binom{d}{2} \times \binom{d}{2}$  matrices in  $\mu$  and  $\nu$  or, equivalently, as one matrix in  $\mu$  and  $\nu$  with vector-like elements living in a  $\binom{d}{2} \times \binom{d}{2}$  dimensional space.

To systematize this picture, it may also be convenient to view  $\mathbf{C}$  as an operator in the tensor product of two spaces. The first,  $\mathcal{H}_1$  is the exterior product  $H_A \wedge H_A$  (or, alternatively  $H_B \wedge H_B$ ). Thus  $\mathcal{H}_1 = \mathbf{C}^{d^2-d/2}$ . The space  $\mathcal{H}_2$  is the space of ‘lists’ of vectors for decomposition of the state. In principle we should allow this space to be infinite dimensional, as one can consider infinite decompositions. However, it is likely that dimension  $d^4$  is sufficient. For example, a separable state can be certainly decomposed into no more than  $d^4$  product states [12]. Similarly, there always exists an optimal decomposition for entanglement of formation containing no more than  $d^4$  components [13].

Matrix  $\mathbf{C}$  viewed as an operator acting on  $\mathcal{H}_1 \otimes \mathcal{H}_2$  has simple transformation rules under (i) change of decomposition and (ii) local unitary transformations of the state. Operations of type (i) transform the preconcurrence matrix according to

$$C^{\mu'\nu'} = \sum_{\mu\nu} U^{\mu'\mu} C^{\mu\nu} U^{\nu'\nu}, \tag{7}$$

with  $\mathbf{U}$  being a unitary matrix changing the decomposition of the state into pure states [14]. This transformation can be represented as

$$\mathbf{C} \rightarrow \mathbf{C}' = \mathbf{I} \otimes \mathbf{U} \mathbf{C} \mathbf{I} \otimes \mathbf{U}^T, \tag{8}$$

where the subscript T stands for transposition. Similarly, a unitary transformation of the local bases

$$|e_{i_1} \otimes f_{i_2}\rangle = \sum_{k_1 k_2} |\hat{e}_{k_1} \otimes \hat{f}_{k_2}\rangle V_{k_1 i_1} W_{k_2 i_2} \tag{9}$$

(matrices  $\mathbf{V}$  and  $\mathbf{W}$  unitary) changes the components of the elements of  $C^{\mu\nu}$  according to

$$\begin{aligned} \hat{C}_{i_1 \wedge j_1; i_2 \wedge j_2}^{\mu\nu} &= \sum_{k_1 l_1 k_2 l_2} V_{i_1 k_1} V_{j_1 l_1} W_{i_2 k_2} W_{j_2 l_2} C_{k_1 \wedge l_1; k_2 \wedge l_2}^{\mu\nu} \\ &= \sum_{k_1 < l_1; k_2 < l_2} (V_{i_1 k_1} V_{j_1 l_1} - V_{i_1 l_1} V_{j_1 k_1}) \\ &\quad \times (W_{i_2 k_2} W_{j_2 l_2} - W_{i_2 l_2} W_{j_2 k_2}) C_{k_1 \wedge l_1; k_2 \wedge l_2}^{\mu\nu}, \end{aligned} \tag{10}$$

which can be represented as

$$\mathbf{C} \rightarrow \hat{\mathbf{C}} = (\mathbf{V} \otimes \mathbf{W}) \otimes \mathbf{IC}(\mathbf{V}^T \otimes \mathbf{W}^T) \otimes \mathbf{I}. \tag{11}$$

### 3. Concurrence and separability

The preconcurrence matrix defined in the previous section sheds some interesting light on the separability of mixed states. Obviously, a given bipartite state  $\varrho$  is separable if there is a decomposition for which all the diagonal elements  $C^{\mu\mu}$  are zero vectors. The non-separable states can then be divided into two classes:

- (a) the states for which there is a pair of local bases such that for at least one  $\kappa_0 = i_1^0 \wedge j_1^0; i_2^0 \wedge j_2^0$ , the diagonal of  $C_{\kappa_0}^{\mu\nu}$  cannot be brought to zero by any transformation (7).
- (b) the states where, for every single component  $\kappa = i_1 \wedge j_1; i_2 \wedge j_2$ , there exists a decomposition with all the diagonal elements  $C_{\kappa}^{\mu\mu}$  zero (different decompositions for different multi-indexes  $\kappa$ ); this property must hold irrespective of the choice of the local bases.

The states in class (a) contain two-qubit entanglement and as such are distillable [15]. Class (b), on the other hand, contains all the bound entangled (BE) states [12, 16]. Indeed, two-qubit entangled states are distillable; hence a BE state cannot contain two-qubit entanglement. A known open question in this context is whether class (b) is equivalent to the BE states or whether it is strictly larger. In [16] it was shown that state  $\varrho$  is distillable if for some number  $k$  state  $\varrho^{\otimes k}$  has two-qubit entanglement. Call such a state  $k$ -copy-pseudo distillable (following the notation of [17]). The question of whether the set of BE states is equal to class (b) can then be rephrased as follows: does  $k$ -copy pseudo-distillability imply one-copy pseudo-distillability? In principle, it might happen that the property of having two-qubit entanglement is not additive; one copy would not contain it, but two or more copies would. For some Werner states there is strong evidence that this is the case [17, 18]. In [19] a possible equivalence of the considered sets was connected with some ‘binarization’ of conditional information in cryptography based on mixed quantum states.

In this context, our preconcurrence matrix allows for a simple argument which shows that rank-2 states are either separable or one-copy pseudo-distillable (for the original proof of non-existence of BE states of rank 2, [20]).

#### 3.1. Rank-2 states are either separable or one-copy pseudo-distillable

Rank-2 states have  $2 \times 2$  preconcurrence matrices. A state which has a decomposition where all the matrices are of the form

$$\mathbf{C}_1 = \begin{bmatrix} 0 & x \\ x & 0 \end{bmatrix} \tag{12}$$

is separable. A candidate for a non-separable and not one-copy pseudo-distillable state must have at least two essentially different preconcurrence matrices. In a decomposition where one of the matrices is of the form (12), there must be another matrix

$$\tilde{\mathbf{C}}_2 = e^{i\varphi} \begin{bmatrix} a e^{i\alpha} & b \\ b & -a e^{-i\alpha} \end{bmatrix}, \quad (13)$$

with all the parameters real and  $a \neq 0$ . This form is necessary since otherwise it would be impossible for transformation (7) to make the diagonal of  $\tilde{\mathbf{C}}_2$  zero. Moreover, a simple phase adjustment in the decomposition of the state can bring  $\alpha$  and  $\varphi$  to zero, without changing  $\tilde{\mathbf{C}}_1$ 's diagonal. With such an adjustment the second matrix becomes

$$\mathbf{C}_2 = \begin{bmatrix} a & b \\ b & -a \end{bmatrix}, \quad (14)$$

with both  $a$  and  $b$  real. Now, a change in the local bases which (up to a normalizing factor) produces

$$\mathbf{C}'_2 = \mathbf{C}_2 + i \begin{bmatrix} 0 & |x| \\ |x| & 0 \end{bmatrix},$$

which shows that the state contains two-qubit entanglement, that is it is distillable. Indeed,  $\mathbf{C}'_2$  is of the form (13) with real non-zero  $a$  and complex  $b$ . Such a matrix has two different singular values. Consequently, no transformation (7) can reduce its trace to zero. This implies two-qubit entanglement.

As a corollary to the above argument, one may notice that a rank-2 state is separable if there exists a two-state decomposition of the state which simultaneously diagonalizes all the  $\mathbf{C}_\kappa$  matrices so that all the matrices are essentially of the same form

$$\mathbf{C}_\kappa = \begin{bmatrix} x_\kappa & 0 \\ 0 & -x_\kappa \end{bmatrix}. \quad (15)$$

Indeed, if separability requires existence of a decomposition where, irrespective of the choice of the local bases, all the  $\mathbf{C}_\kappa$  matrices are of the form (12), then transformation (7) with

$$\mathbf{U} = \mathbf{U}_q = \frac{1}{2^{1/2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \quad (16)$$

transforms them into the form (15).

Analysis of separability of states of rank higher than two appears to be more difficult. In particular, an attempt to follow Wootters' minimization procedure for the expectation value of the concurrence's norm is not simple since there is no guarantee that transformation (8) can diagonalize matrix  $\mathbf{C}$  (note that the elements of  $\mathbf{C}$  are vectors while the elements of  $\mathbf{U}$  are numbers). One can, nevertheless, diagonalize  $\mathbf{D} = \text{Tr}_{\mathcal{H}_1}(\mathbf{C}\mathbf{C}^\dagger)$ . This leads to some simplifications in special cases, for example when diagonal  $\mathbf{D}$  implies diagonal  $\mathbf{C}$ . Nevertheless, at the moment, we do not have any general results for states of rank higher than 2.

#### 4. Biconcurrence

Bearing in mind the difficulties, one may try to look at the generalized concurrence from a somewhat different perspective. For two qubits, preconcurrence

rence can be viewed as a bilinear form  $\mathbf{C}(\psi, \phi)$  which distinguishes between product vectors and entangled vectors. It satisfies the following crucial condition.

**Condition 1:**  $\mathbf{C}(\psi, \psi) = 0$  if and only if  $\psi$  is a product vector.

In passing, one may note that a form which satisfies condition 1 cannot be linear in one argument and antilinear in the other, since a linear–antilinear form can be written as

$$\mathbf{C}(\psi, \phi) = \langle \psi | A \phi \rangle, \tag{17}$$

where  $A$  is a linear operator acting on space  $\mathcal{H}$ . However, form (17) which vanishes on all the product vectors, vanishes everywhere, thus violating condition 1. Consequently, the form must be bilinear (or biantilinear; it does not matter which). In this context, Wootters’ concurrence defines a good form for  $\mathcal{H} = \mathbf{C}^2 \otimes \mathbf{C}^2$ . It is

$$\mathbf{C}(\psi, \phi) = \langle \tilde{\psi} | \phi \rangle. \tag{18}$$

Wootters’ preconcurrence matrix is then simply

$$C^{\mu\nu}(\varrho) = \mathbf{C}(\psi_\mu, \psi_\nu). \tag{19}$$

Unfortunately, from [8], in higher dimensions there does not exist a bilinear form satisfying condition 1. A possible way to generalize Wootters’ concurrence can then be to look for a four-argument form  $\mathbf{B}(\psi, \phi, \kappa, \theta)$  which would satisfy the following condition.

**Condition 1’:**  $\mathbf{B}(\psi) \equiv \mathbf{B}(\psi, \psi, \psi, \psi) = 0$  iff  $\psi$  is a product vector.

A possible form satisfying condition 1’, linear in two arguments and antilinear in the two others is closely related to the Rungta *et al.* concurrence [9] and to our preconcurrence matrix. For instance, one can take a slightly simplified version of concurrence in [9] as a departure point and define

$$\mathbf{B}(\psi) = -\langle \psi | \mathbf{I} \otimes \Lambda(|\psi\rangle\langle\psi|) | \psi \rangle. \tag{20}$$

where  $\Lambda$  is the positive map used in the reduction criterion of separability [20]:  $\Lambda(A) = \text{Tr}(A)\mathbf{I} - A$ .

One finds that  $\mathbf{B}(\psi) = 1 - \text{Tr}\varrho^2$ , where  $\varrho$  is a reduction of  $\psi$ . It is then clear that  $\mathbf{B}$  satisfies condition 1’. The corresponding biconcurrence matrix is then

$$B^{\mu\nu mn} = \mathbf{B}(\psi_\mu, \psi_\nu, \psi_m, \psi_n) = -\langle \psi_\mu | \mathbf{I} \otimes \Lambda(|\psi_\nu\rangle\langle\psi_m|) | \psi_n \rangle. \tag{21}$$

After some algebra this can be rewritten as

$$B^{\mu\nu mn} = \langle \psi_\mu | \psi_\nu \rangle \langle \psi_m | \psi_n \rangle - \text{Tr}([\psi_\mu]^\dagger [\psi_\nu] [\psi_m]^\dagger [\psi_n]), \tag{22}$$

which is simply a partial contraction of a product of preconcurrence matrix with its complex conjugation:

$$B^{\mu\nu mn} = \frac{1}{4} \sum_{i\wedge j, k\wedge l} C_{i\wedge j; k\wedge l}^{\mu\nu} \left( C_{i\wedge j; k\wedge l}^{m\mu} \right)^*. \tag{23}$$

Biconcurrence is invariant under local unitary rotations of the state. Changes in the state’s decomposition, on the other hand, transform biconcurrence as follows:

$$\tilde{\mathbf{B}}^{\mu\nu mn} = \sum_{\alpha, \beta, a, b} (U^{\mu\alpha})^* (U^{ma})^* B^{\alpha\beta ab} U^{\nu\beta} U^{nb}. \quad (24)$$

If we treat matrix  $\mathbf{B}$  as an operator acting on a tensor product of Hilbert spaces with Greek (italic) indices for first (second) space, we obtain

$$\tilde{\mathbf{B}} = \mathbf{U}^* \otimes \mathbf{U}^* \mathbf{B} (\mathbf{U}^*)^\dagger \otimes (\mathbf{U}^*)^\dagger. \quad (25)$$

One can see that matrix  $\mathbf{B}$  contains the whole information about a possible separability of state  $\rho$ . Moreover, irrespective of the decomposition, the elements on the main diagonal of  $\mathbf{B}$  are real and non-negative. Therefore, in terms of biconcurrence, separability is equivalent to the existence of a unitary  $\mathbf{U}$  such that, in equation (25),

$$\text{tr}(\tilde{\mathbf{B}}) = 0, \quad (26)$$

where  $\text{tr}$  with an initial lower-case  $t$  is here understood as the sum of the elements on the main diagonal:

$$\text{tr} \tilde{\mathbf{B}} = \sum_{\mu} \tilde{B}^{\mu\mu\mu\mu}. \quad (27)$$

Note that the elements  $\tilde{B}^{\mu\mu\mu\mu}$  are always non-negative. Therefore it suffices to minimize equation (26) over unitary matrices  $\mathbf{U}$  and to check whether the minimum is zero.

Within the picture of  $\mathbf{B}$  acting on a product of Hilbert spaces, one can express the condition as follows:

$$\min_{\mathbf{U}} [\text{Tr}(\mathbf{U} \otimes \mathbf{U} \mathbf{P} \mathbf{U}^\dagger \otimes \mathbf{U}^\dagger \mathbf{B})] = 0, \quad (28)$$

where  $\mathbf{P} = \sum_i |ii\rangle\langle ii|$  with  $|ij\rangle$  being the standard product basis.

Condition (26) seems to be quite simple, and we hope that it will lead to a more operational condition for separability.

## 5. Conclusions

In conclusion, we argue that the multidimensional generalizations of concurrence which we have introduced in this contribution put the question of separability of bipartite quantum states in a new perspective.

First, we introduced the concept of a preconcurrence matrix. The matrix was designed to distinguish between the contributions to the entanglement which embrace pairs of different two-dimensional subspaces of the bipartite system. In this way, our preconcurrence matrix contained all the information necessary to identify separability of a given state. Nevertheless, its dependence on the particular choice of the local basis made it often difficult to analyse in detail.

Therefore, we also generalized the concept of concurrence in another direction and abandoned the requirement for it to be a second-order object in the state's ensemble. We arrived at the concept of biconcurrence matrix. This matrix is of the fourth order in the state's ensemble; however, because of this, it is invariant under local unitaries. Biconcurrence can be easily derived from a given bipartite state directly. It can also be constructed by a suitable contraction out of our preconcurrence matrix. The resulting separability condition is probably the easiest possible from the algebraic point of view.



Regarding a complete characterization of entanglement, on the other hand, our generalizations of concurrence matrix may not be enough. The main reason for this is that in order to specify the singular values of  $[\psi]$ , in addition to the length of the preconcurrence defined in equation (4), one needs the lengths of all its trilinear,  $\dots$ ,  $d$ -linear analogues. We hope to return to this point in the near future.

## Acknowledgments

P.B. is partially supported by Svenska Institutet, project ML2000. In addition, P.B. acknowledges stimulating discussions with Richard Bonner and Benjamin Baumslag. M.H., P.H. and R.H. are supported by the Polish Committee for Scientific Research, contract 2 P03B 103 16 and by UE project EQUIP, contract IST-1999-11053.

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