Unextendible Product Bases and Bound Entanglement

Charles H. Bennett,[1] David P. DiVincenzo,[1] Tal Mor,[2] Peter W. Shor,[3] John A. Smolin,[1] and Barbara M. Terhal[4]
[1]*IBM, T. J. Watson Research Center, Yorktown Heights, New York 10598*
[2]*DIRO, Université de Montréal, Canada*
and Department of Electrical Engineering, UCLA, Los Angeles, California 90095-1594
[3]*AT&T Labs-Research, Florham Park, New Jersey 07932*
[4]*ITF, UvA, Valckenierstraat 65, 1018 XE Amsterdam*
and CWI, Kruislaan 413, 1098 SJ Amsterdam, The Netherlands
(Received 20 August 1998; revised manuscript received 16 February 1999)

An *unextendible product basis* (UPB) for a multipartite quantum system is an incomplete orthogonal product basis whose complementary subspace contains no product state. We give examples of UPBs, and show that the uniform mixed state over the subspace complementary to any UPB is a *bound entangled* state. We exhibit a tripartite $2 \times 2 \times 2$ UPB whose complementary mixed state has tripartite entanglement but no bipartite entanglement, i.e., all three corresponding 2×4 bipartite mixed states are unentangled. We show that members of a UPB are not perfectly distinguishable by local positive operator valued measurements and classical communication. [S0031-9007(99)09360-6]

PACS numbers: 03.67.Hk, 03.65.Bz, 89.70.+c

Einstein, Podolsky, and Rosen [1] first highlighted the nonlocal features of entangled (or nonfactorizable) quantum states of two separated particles. Bell showed that this entanglement implied a true nonlocality, or lack of local realism in quantum mechanics [2]. But it is now clear that there are other manifestations of quantum nonlocality that go beyond entanglement [3]. In this Letter we uncover various nonlocal properties of some simple m-party sets of quantum states that involve only product (i.e., unentangled) states.

We present detailed examples of two-party and the three-party sets of orthogonal product states that are *unextendible*, meaning that no further product states can be found orthogonal to all the existing ones in a given Hilbert space. We call such a set an unextendible product basis (or UPB), and show that unextendibility gives rise to two other recently discovered and not yet well-understood quantum phenomena; (1) the mixed state on the subspace complementary to a UPB is a *bound entangled* state [4,5], i.e., an entangled mixed state from which no pure entanglement can be distilled. We thus provide the first systematic way of constructing bound entangled states, a task which had been exceedingly difficult. (2) The states comprising a UPB are *locally immeasurable* [3], i.e., an unknown member of the set cannot be reliably distinguished from the others by local measurements and classical communication. Though sufficient, unextendibility is not a necessary condition for either of these phenomena, as there exist bound entangled states [4,5] not associated with any UPB, and locally immeasurable sets of states which are not only extendible, but capable of being extended all the way to a complete orthogonal product basis on the entire Hilbert space [3].

Definition 1.—Consider a multiparticle quantum system $\mathcal{H} = \bigotimes_{i=1}^{m} \mathcal{H}_i$ with m parts of respective dimension $d_i, i = 1 \ldots, m$. A (incomplete orthogonal) product basis (PB) is a set S of pure orthogonal product states spanning a proper subspace $\mathcal{H}_S$ of $\mathcal{H}$. A UPB is a PB whose complementary subspace $\mathcal{H} - \mathcal{H}_S$ contains no product state.

To illustrate how a PB can fail to be extendible, consider the following two sets of five states on 3×3 (two qutrits):

(1) Let $\vec{v}_0, \vec{v}_1, \ldots, \vec{v}_4$ be five vectors in real three-dimensional space forming the apex of a regular pentagonal pyramid, the height h of the pyramid being chosen such that nonadjacent vectors are orthogonal (cf. Fig. 1). The vectors are

$$\vec{v}_j = N\left(\cos\frac{2\pi j}{5}, \sin\frac{2\pi j}{5}, h\right), \qquad j = 0, \ldots, 4, \quad (1)$$

with $h = \frac{1}{2}\sqrt{1 + \sqrt{5}}$, and $N = 2/\sqrt{5 + \sqrt{5}}$. Then the following five states in 3×3 Hilbert space form a UPB, henceforth denoted PYRAMID

$$|\psi_j\rangle = |\vec{v}_j\rangle \otimes |\vec{v}_{2j \bmod 5}\rangle, \qquad j = 0, \ldots, 4. \quad (2)$$

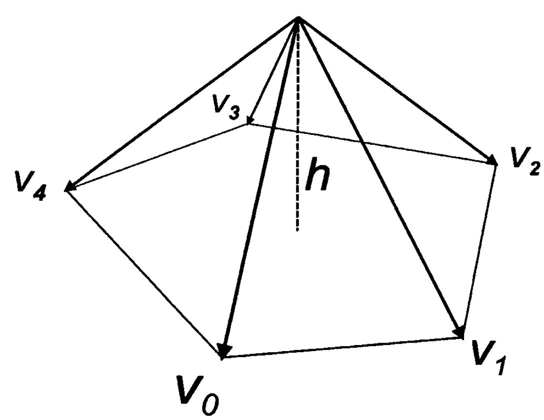

FIG. 1. PYRAMID vectors in real 3-space. The height h is chosen so that $v_0 \perp v_{2,3}$, etc.

To see that these five states form a UPB, note first that they are mutually orthogonal: states whose indices differ by 2 mod 5 are orthogonal for the first party ("Alice"); those whose indices differs by 1 mod 5 are orthogonal for the second party ("Bob"). For a new product state to be orthogonal to all the existing ones, it would have to be orthogonal to at least three of Alice's states or at least three of Bob's states. However this is impossible, since any three of the vectors $\vec{v}_i$ span the full three-dimensional space in which they live. Therefore the entire four-dimensional subspace complementary to PYRAMID contains no product state.

(2) The following five states on 3×3 form a UPB henceforth denoted TILES

$$
\begin{aligned}
|\psi_0\rangle &= \frac{1}{\sqrt{2}}\,|0\rangle(|0\rangle - |1\rangle)\,, \\
|\psi_2\rangle &= \frac{1}{\sqrt{2}}\,|2\rangle(|1\rangle - |2\rangle)\,, \\
|\psi_1\rangle &= \frac{1}{\sqrt{2}}\,(|0\rangle - |1\rangle)|2\rangle\,, \\
|\psi_3\rangle &= \frac{1}{\sqrt{2}}\,(|1\rangle - |2\rangle)|0\rangle\,, \\
|\psi_4\rangle &= \tfrac{1}{3}\,(|0\rangle + |1\rangle + |2\rangle)(|0\rangle + |1\rangle + |2\rangle)\,.
\end{aligned}
\tag{3}
$$

Note that the first four states are the interlocking tiles of [3], and the fifth state works as a "stopper" to force the unextendibility.

In both examples, any subset of three vectors on either side spans the three-dimensional space of that party, preventing any new vector from being orthogonal to all the existing ones. We formalize this observation by giving the necessary and sufficient condition for extendibility of a PB:

Lemma 1: Let $S = \{(\psi_j \equiv \bigotimes_{i=1}^{m} \varphi_{i,j})\colon j = 1,\dots,n\}$ be an incomplete orthogonal PB of an m-partite quantum system. Let P be a partition of S into m disjoint subsets: $S = S_1 \cup S_2 \cup, \dots, S_m$. Let $r_i = \mathrm{rank}\{\varphi_{i,j}\colon \psi_j \in S_i\}$ be the local rank of subset S_i as seen by the ith party. Then S is extendible if and only if there exists a partition P such that for all $i = 1,\dots,m$, the local rank r_i of the ith subset is less than the dimension d_i of the ith party's Hilbert space.

Proof: Imagine that the parties $i = 1,\dots,m$ allocate among themselves the job of being orthogonal to a new product state we are trying to add. The new state will be orthogonal to all the existing ones if a partition can be found such that the new state is orthogonal to all the states in S_1 for party 1, all the states in S_2 for party 2, and so on through S_m. Clearly this can be done (e.g., by local Gram-Schmidt orthogonalization for each party) if each of the sets S_i has local rank r_i less than the dimensionality d_i of the ith party's Hilbert space. Conversely, if for every partition, at least one of the sets S_i has full rank, equal to d_i, there is no way to choose a new product state orthogonal to all existing states; thus the original set is not extendible.

The lemma provides a simple lower bound on the number of states n in a UPB,

$$n \geq \sum_i (d_i - 1) + 1\,, \tag{4}$$

since, for smaller n, one can partition S into sets of size $|S_i| \leq d_i - 1$ and thus $r_i < d_i$ for all m parties.

As noted earlier, UPBs provide a way to construct bound entangled (BE) states, i.e., entangled mixed states from which no pure entanglement can be distilled [4,5]. It was shown in [5] that if a bipartite density matrix ρ remains positive semidefinite under the partial transposition condition (PT) of Peres [6], then ρ cannot have distillable entanglement. We then say that ρ has positive partial transposition (PPT).

Theorem 1: The state that corresponds to the uniform mixture on the space complementary to a UPB $\{\psi_i\colon i = 1,\dots,n\}$ in a Hilbert space of total dimension D

$$\overline{\rho} = \frac{1}{D - n}\left(\mathbf{1} - \sum_{j=1}^{n} |\psi_j\rangle\langle\psi_j|\right) \tag{5}$$

is a bound entangled state.

Proof: By definition, the space complementary to a UPB contains no product states. Therefore $\overline{\rho}$ is entangled. If the UPB is bipartite then $\overline{\rho}$ is PPT by construction: The identity is invariant under PT and the product states making up the UPB are mapped onto another set of orthogonal product states. Therefore $PT(\overline{\rho})$ is another density matrix, and thus positive semidefinite. For the case of many parties the PPT condition cannot be used directly, so we use the above argument to show that every bipartite partitioning of the parties is PPT. Thus no entanglement can be distilled across any bipartite cut. If any pure global entanglement could be distilled it could be used to create entanglement across a bipartite cut. Since $\overline{\rho}$ is entangled and is not distillable, it is bound entangled.

We compute that the state complementary to the TILES UPB has a (bound) entanglement of the formation [7] of 0.213726 ebits and the PYRAMID UPB has an entanglement of the formation of 0.232635 ebits. These numbers are surprisingly large, considering that the maximal entanglement for any state in 3×3 is $\log_2 3 \approx 1.585$ ebits.

An example of a UPB involving three parties, A, B, and C, each holding a qubit, is the set

$$\{|0,1,+\rangle, |1,+,0\rangle, |+,0,1\rangle, |-,-,-\rangle\}\,, \tag{6}$$

with $\pm = (|0\rangle \pm |1\rangle)/\sqrt{2}$. One can see using Lemma 1 that there is no product state orthogonal to these four states, which we will henceforth call the SHIFTS UPB. This UPB can be simply generalized to a UPB over any number of parties, each with a one qubit Hilbert space (see [8]).

The complementary state to the SHIFTS constructed by Eq. (5) has the curious property that not only is it two-way PPT, it is also two-way separable, i.e., the entanglement across any split into two parties is zero. This solves the main problem left open in [9] and surprisingly refutes a natural conjecture made there. To show that the entanglement between A and BC is zero, we write $a = |1,+\rangle$, $b = |+,0\rangle$, $v = |0,1\rangle$, and $d = |-,-\rangle$. Note that these are just the B and C parts of the four states in Eq. (6), and that $\{a,b\}$ are orthogonal to $\{c,d\}$. Consider the vectors $a^\perp$ and $b^\perp$ in the span(a,b) and the vectors $c^\perp$ and $d^\perp$ in the span(c,d). Now, we can complete the original set of vectors to a full product basis between A and BC with the states $\{|0,a^\perp\rangle, |1,b^\perp\rangle, |+,c^\perp\rangle, |-,d^\perp\rangle\}$. By the symmetry of the states, this is also true for the other splits.

We now consider another nonlocal property of UPBs, their relation to local immeasureability. In this context, a useful notion, more general than unextendibility, is *uncompletability*, an uncompletable product basis being one that might be able to be extended by one or more states, but cannot be completed to a full orthogonal product basis on the entire Hilbert space. Another concept we will need is that of uncompletability even in a larger Hilbert space with local extensions, where each party's space is extended from $\mathcal{H}_i$ to $\mathcal{H}_i \oplus \mathcal{H}_i'$. We have the following simple fact about UPBs:

Lemma 2: A UPB is not completable even in a locally extended Hilbert space.

Proof: If a set of states is completable in a locally extended Hilbert space, then its complement space in the extended Hilbert space is separable. By local projections the uniform state on the complementary space in the extended Hilbert space can be projected onto the complementary space in the original Hilbert space. This state is also separable since local projections do not create entanglement. But we have a contradiction since the state complementary to a UPB is entangled (Theorem 1).

We are now ready to show that uncompletability with local Hilbert space extensions is a sufficient condition for a set of orthogonal product states not to be perfectly distinguishable by any sequence of local positive operator valued measurements (POVMs) even with the help of classical communication among the observers. This form of local immeasurability was first studied in [3]. To obtain a finite bound on the level of distiguishability of such sets (as was done for the sets in [3]) requires additional work and will be presented in [8].

Lemma 3: Given a set S of orthogonal product states on $\mathcal{H} = \bigotimes_{i=1}^m \mathcal{H}_i$ with $\dim \mathcal{H}_i = d_i, i = 1,\ldots,m$. If the set S is exactly measurable by local von Neumann measurements and classical communication, then it is completable in $\mathcal{H}$. If S is exactly measurable by local POVMs and classical communication, then the set can be completed in some extended space $\mathcal{H}' = \bigotimes_{i=1}^m (\mathcal{H}_i \oplus \mathcal{H}_i')$.

Proof: We show how a local von Neumann measurement protocol leads directly to a way to complete the set S. At some stage of their protocol, the parties (1) may have been able to eliminate members of the original set of states S, and (2) they may have mapped, by performing their von Neumann measurements, the remaining set of orthogonal states into a new set of *orthogonal* states S'. Determining which member they have in this new set uniquely determines which state of S they started with. At this stage, party i_0 performs an l-outcome von Neumann measurement which is given by a decomposition of the remaining Hilbert space $\mathcal{K} = \mathcal{K}_{\rm else} \otimes \mathcal{K}_{i_0}$ with $\mathcal{K}_{\rm else} = \bigotimes_{j \neq i_0} \mathcal{K}_j$, into a set of l orthogonal subspaces, $\mathcal{K}_{\rm else} \otimes P_1 \mathcal{K}_{i_0}, \ldots, \mathcal{K}_{\rm else} \otimes P_l \mathcal{K}_{i_0}$.

If a state in S' lies in one of these subspaces, it will be unchanged by the measurement. If a state $|\alpha\rangle \otimes |\beta\rangle$, where $|\alpha\rangle \in \mathcal{K}_{\rm else}$, is not contained in one of the subspaces, it will be projected onto one of the states $\{|\alpha\rangle \otimes P_1|\beta\rangle, |\alpha\rangle \otimes P_2|\beta\rangle, \ldots, |\alpha\rangle \otimes P_l|\beta\rangle\}$. Let S'' be this new projected set of states, containing both the unchanged states in S' as well as the possible projections of the states in S'. If one of the subspaces does not contain a member of S', it can be completed directly. For the other subspaces, let us assume that each of them can be completed individually with product states orthogonal to members of S''. In this way we have completed the projected S' on the full Hilbert space $\mathcal{K}$, as these orthogonal-subspace completions are orthogonal sets and they are a decomposition of $\mathcal{K}$. However, we have now completed the set S'' rather than the set S'. Fortunately, one can replace the projected states $|\alpha\rangle \otimes P_1|\beta\rangle, \ldots, |\alpha\rangle \otimes P_l|\beta\rangle$ by the original state $|\alpha\rangle \otimes |\beta\rangle$ and $l-1$ orthogonal states by making l linear combinations of the projected states. They are orthogonal to all other states as each $|\alpha\rangle \otimes P_i|\beta\rangle$ was orthogonal, and they can be made mutually orthogonal as they span an l-dimensional space on the i_0 side. Thus at each round of measurement, a completion of the set of states S' is achieved assuming a completion of the subspaces determined by the measurement.

The tree of nested subspaces will always lead to a subspace that contains only a single state of the set, as the measurement protocol was able to tell the states in S apart exactly. But such a subspace containing only one state can easily be completed and thus, by induction, we have proved that the original set S can be completed in $\mathcal{H}$.

Finally, we note that a POVM is simply a von Neumann measurement in an extended Hilbert space (this is Neumark's theorem (cf. [10]). Thus any sequence of POVMs implementable locally with classical communications is a sequence of local von Neumann measurements in extended Hilbert spaces and the preceding argument applies, leading to a completion in $\mathcal{H}'$.

Theorem 2: Members of a UPB are not perfectly distinguishable by local POVMs and classical communication.

Proof: If the UPB were measurable by POVMs, it would be completable in some larger Hilbert space by Lemma 3. But this is in contradiction with Lemma 2.

We now give an example of a PB that is measurable by local POVMs, but not by local von Neumann measurements, which will also serve to illustrate the proofs just given. The set is in a Hilbert space of dimension 3×4.

Consider the set $\vec{v}_j \otimes \vec{w}_j$, $j = 0, \ldots, 4$ with $\vec{v}_j$ the states of the PYRAMID UPB as in Eq. (1) with $\vec{w}_j$ defined as

$$\vec{w}_j = N[\sqrt{\cos(\pi/5)}\,\cos(2j\pi/5), \sqrt{\cos(\pi/5)}\,\sin(2j\pi/5), \sqrt{\cos(2\pi/5)}\,\cos(4j\pi/5), \sqrt{\cos(2\pi/5)}\,\sin(4j\pi/5)], \tag{7}$$

with normalization $N = \sqrt{2/\sqrt{5}}$. Note that $\vec{w}_j^T \vec{w}_{j+1} = 0$ (addition mod 5). One can show that this set, albeit extendible on 3×4, is not *completable*: One can at most add three vectors such as $\vec{v}_0 \otimes (\vec{w}_0, \vec{w}_1, \vec{w}_4)^\perp$, $\vec{v}_3 \otimes (\vec{w}_2, \vec{w}_3, \vec{w}_4)^\perp$, and $(\vec{v}_0, \vec{v}_3)^\perp \otimes (\vec{w}_1, \vec{w}_2, \vec{w}_4)^\perp$.

The POVM measurement that is performed by Bob on the four-dimensional side has five projector elements, each projecting onto a vector $\vec{u}_j = N(-\sin(2j\pi/5), \cos(2j\pi/5), -\sin(4j\pi/5), \cos(4j\pi/5))$ with $j = 0, \ldots, 4$, and normalization $N = 1/\sqrt{2}$. Note that $\vec{u}_0$ is orthogonal to vectors $\vec{w}_0$, $\vec{w}_2$, and $\vec{w}_3$, or, in general, $\vec{u}_i$ is orthogonal to $\vec{w}_i, \vec{w}_{i+2}, \vec{w}_{i+3}$ (addition mod 5). This means that upon Bob's POVM measurement outcome, three vectors are excluded from the set; then the remaining two vectors on Alice's side, $\vec{v}_{i+1}$ and $\vec{v}_{i+4}$, are orthogonal and can thus be distinguished.

The completion of this set is particularly simple. Bob's Hilbert space is extended to a five-dimensional space. The POVM measurement can be extended as a projection measurement in this five-dimensional space with orthogonal projections onto the states $\vec{x}_i = (\vec{u}_i, 0) + \frac{1}{2}(0,0,0,0,1)$. Then a completion of the set in 3×5 are the following ten states:

$$\begin{aligned}
&(\vec{v}_1, \vec{v}_4)^\perp \otimes \vec{x}_0, && \vec{v}_0 \otimes [\vec{w}_0^\perp \in \mathrm{span}(\vec{x}_4, \vec{x}_1)],\\
&(\vec{v}_0, \vec{v}_2)^\perp \otimes \vec{x}_1, && \vec{v}_1 \otimes [\vec{w}_1^\perp \in \mathrm{span}(\vec{x}_0, \vec{x}_2)],\\
&(\vec{v}_1, \vec{v}_3)^\perp \otimes \vec{x}_2, && \vec{v}_2 \otimes [\vec{w}_2^\perp \in \mathrm{span}(\vec{x}_1, \vec{x}_3)],\\
&(\vec{v}_2, \vec{v}_4)^\perp \otimes \vec{x}_3, && \vec{v}_3 \otimes [\vec{w}_3^\perp \in \mathrm{span}(\vec{x}_2, \vec{x}_4)],\\
&(\vec{v}_0, \vec{v}_3)^\perp \otimes \vec{x}_4, && \vec{v}_4 \otimes [\vec{w}_4^\perp \in \mathrm{span}(\vec{x}_3, \vec{x}_0)],
\end{aligned} \tag{8}$$

Although UPBs provide an easy way to construct a wide variety of bound entangled states, not all bound entangled states can be constructed by this method. In [4], a 2×4 state with bound entanglement was presented. However, our construction fails for any $2 \times n$ as there is no UPB in $2 \times n$ for any n. This follows from Theorem 2 and the fact that any set of orthogonal product states on $2 \times n$ is locally measurable. The measurement is a three round protocol. Assume Alice has the two-dimensional side. We write the set of states as $\{|\alpha_1\rangle \otimes |\beta_1\rangle, \ldots, |\alpha_k\rangle \otimes |\beta_k\rangle\}$. Alice can divide the states $|\alpha_1\rangle, \ldots, |\alpha_k\rangle$ on her side in sets P_i that have to be mutually orthogonal on Bob's side, namely, $P_1 = \{|\alpha_1\rangle, |\alpha_1\rangle, \ldots, |\alpha_1\rangle^\perp, \ldots\}, \ldots, P_i = \{|\alpha_i\rangle, |\alpha_i\rangle, \ldots, |\alpha_i\rangle^\perp\}$, etc., as $|\alpha_i\rangle$ and $|\alpha_j\rangle$ for $i \neq j$ are neither orthogonal nor identical. Note that $|\alpha_i\rangle$ or $|\alpha_i\rangle^\perp$ can be repeated, but if they are, these states should be orthogonal on Bob's side. Now Bob can do a projection measurement that singles out a subspace associated with P_i. After Bob sends this information, the label i to Alice, she does a measurement that distinguishes $|\alpha_i\rangle$ from $|\alpha_i\rangle^\perp$. Then Bob can finish the protocol by measuring among the orthogonal repeaters.

Thus the following implications hold among properties of an incomplete, orthogonal product basis: unextendible $\Rightarrow$ complementary mixed state is BE $\Rightarrow$ not completable even in a locally extended Hilbert space $\Rightarrow$ not measurable exactly by local POVMs, and classical communication $\Rightarrow$ preparation process $|j\rangle \rightarrow |\psi_j\rangle$ is thermodynamically irreversible if carried out locally (cf. [3]).

These constructions, relating entanglement to several other kinds of nonlocality and irreversibility, may help illuminate some of the following questions: How can BE states be used in quantum protocols—for example, to perform otherwise nonlocal separable superoperators [3]? Can local hidden variable descriptions of BE states be ruled out? What relation is there between the irreversibility implicit in the definition of BE states and the thermodynamic irreversibility [3] of preparation of local immeasurable sets of states complementary to them?

We acknowledge the support of Elsag-Bailey and the Institute for Scientific Interchange during the 1998 Quantum Computation Workshop. C. H. B., D. P. D., and J. A. S. are grateful for support by the U.S. Army Research Office under Contract No. DAAG55-98-C-0041. The work of T. M. was supported in part by Grant No. 961360 from the Jet Propulsion Lab.

[1] A. Einstein, B. Podolsky, and N. Rosen, Phys. Rev. **47**, 777 (1935).
[2] J. S. Bell, Physics (Long Island City, N.Y.) **1**, 195 (1964).
[3] C. H. Bennett, D. P. DiVincenzo, C. A. Fuchs, T. Mor, E. Rains, P. W. Shor, J. A. Smolin, and W. K. Wootters, Phys. Rev. A **59**, 1070 (1999).
[4] P. Horodecki, Phys. Lett. A **232**, 333 (1997).
[5] M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Rev. Lett. **80**, 5239 (1998).
[6] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).
[7] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, Phys. Rev. A **54**, 3824 (1996).
[8] C. H. Bennett, D. P. DiVincenzo, T. Mor, P. W. Shor, J. A. Smolin, and B. M. Terhal (to be published).
[9] G. Brassard and T. Mor, in *Proceedings of the 1st NASA Quantum Computing & Quantum Communications, QCQC '98*, Lecture Notes in Computer Science Vol. 1509 (Springer-Verlag, Berlin, 1999).
[10] A. Peres, *Quantum Theory: Concepts and Methods* (Kluwer Academic Publishers, Dordrecht, The Netherlands, 1993).