influence the course of events. While the average reader may be amused—I am afraid that science will suffer. News should be reported fully and problems not be swept under the rug, but there is a line between reporting facts and inserting editorial opinion; in this case I feel that the line has been crossed.

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Estimating SURA's cost

The article on the SURA accelerator in September (page 55) states that the project "lacks a definite design and detailed cost estimate." As our company prepared the estimate for the accelerator, I would like to respond to this criticism.

We have prepared estimates for the first SLAC and Fermilab accelerators as well as the LAMPF linear accelerator on which approvals of these projects were based. In my opinion, the SURA design was at least as complete and more certain to operate essentially as proposed than any of the abovementioned projects.

Although the design output requires improved klystrons, such expectations are typical of accelerator project proposals. If the required improvements cannot be made, a larger number of lower-power tubes could be used or a lower but still satisfactory current output accepted.

The overall cost of large accelerator laboratories is typically two to three times the cost of the accelerator. These additional costs depend, to a considerable extent, on the amenities provided and the scale of the administrative organization to be accommodated. They also depend on the cost of the equipment required to conduct the experiments and how much of that cost is included in the cost of the project. These items may require further definition, but I see no reason for re-estimating the cost of the accelerator itself as long as the existing design is not significantly changed.

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Molecular rotation spectra

The "Search and discovery" section of PHYSICS TODAY should be the place to find carefully chosen, scrupulously edited, and appropriately referenced accounts of the most important recent developments in physics. It is read by nonexperts in the field under report, and it is presumed to be objective. "High-spin molecular rotation spectra are surprisingly simple" (July, page 17), which purports to be an account of the enormous theoretical progress that has been made toward the understanding of the vibration–rotation spectra of polyatomic molecules in the past few years, fails on all these counts.

Over the past 20 years, important advances have been made in the understanding of the vibration–rotation spectra of polyatomic molecules. Among the most important general advances has been work on molecular symmetry by Jon T. Hougen and H. C. Longuet-Higgins, and the simplification of the Hamiltonian and the discovery of the correct way to treat centrifugal distortions when analyzing spectra, both by J. K. G. Watson. None of this has been reported in "Search and discovery." The clustering of the rotational energy levels of spherical top molecules at high angular momenta (the sole topic of the July 1984 article) is an interesting, albeit rather specialized, development for which William Harter and Chris Patterson can take some credit. However, all the credit for its discovery and classical interpretation must go to A. J. Dorney and Watson.[1] This reference is not given in the article and only a passing mention (with incorrect initials for Watson) is made to it. Also, much is made of ortho–para interactions ("the violation of a hitherto sacrosanct selection rule") as if this were a new theoretical development; this is untrue and has been well understood for a great many years. It was first observed[2] by Irving Ozier in 1971.

It is only natural to be enthusiastic about one's research, and it can easily happen that one has an inflated view of its importance. Harter and Patterson can certainly be forgiven for presenting their research in an overly enthusiastic manner bordering on Madison Avenue, but the editors of PHYSICS TODAY must take a more balanced view.

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WILLIAM G. HARTER COMMENTS: Bertram Schwarzschild, the author of the July "Search and discovery" article, did solicit and use comments from a number of experts in the field of molecular spectroscopy, including Hougen. The resulting article was judged to be a fairly balanced account of retical developments that help in visualizing complex dynamics and spectra that arise from solving various molecular Hamiltonians. It was not intended to be an exhaustive review of the

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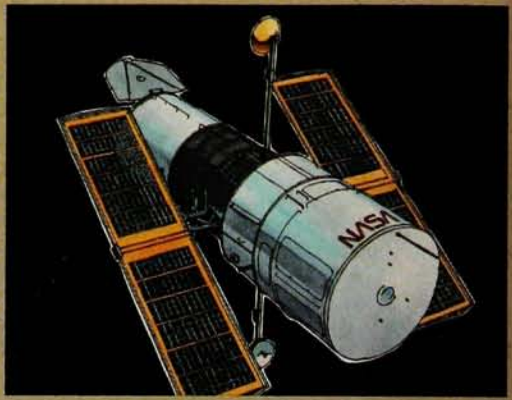

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algebraic *development* of Hamiltonians and molecular symmetry theory. To do so would require a lengthy discussion of the work of Jahn, Karl T. Hecht, Moret-Bailey, J. D. Louck and many others besides Watson. (The RE surface example shown in the figures represents the quantizing trajectories for one of Hecht's Hamiltonians). Instead, the article described an approach that provides new insight into the symmetry properties of eigenstates and dynamics of non-stationary states governed by various molecular Hamiltonians.

References to the paper by Dorney and Watson are included in all our publications on the subject of clustering, and we included it in our comments to the author. However, it is a policy of the editors to list only very recent references in news stories. Also deleted was any mention of K. R. Lea, M. J. M. Leask, and W. P. Wolf, who discovered clusters in related computer studies of atomic angular momentum levels ten years before Dorney and Watson. (Certain types of clusters with quenched angular momenta had also been seen in computer models of ion crystal field spectra even before that.) However, Schwarzschild's article does emphasize Dorney and Watson's published ideas on clustering. In fact, it overstates rather than understates their contribution, since the subject of rotational tunneling mechanism and resulting superfine splitting was not discussed in their paper. The introduction of semiclassical (vs. purely classical) models of rotational motion is also a new development and is based upon a better understanding of clustering.

To say this is a rather specialized development does an injustice to a large and growing number of sophisticated experiments in which clustering and related effects play a predominant role. One of these effects is cluster-induced hyperfine mixing, in which the standard symmetry species are so strongly mixed that they cease to be valid quantum labels. (The effect is analogous to cases in atomic spectra in which nearby levels in the same atom belong to different j–j and L–S coupling limits.) This is to be distinguished from a *weak*, or perturbative, mixing of species, which was recognized by Gerhard Herzberg. He included the clause "... since the coupling of the nuclear spin with the rest of the molecule is so extremely weak ..." when stating the prevailing rule forbidding interspecies transitions. Ozier and others have observed the results of a weak mixing perturbation in methane spectra. Their effects involved the two $J=2$ species in the presence of Stark and Zeeman fields. The Bordés have observed qualitatively and quantitatively different effects associated with a major readjustment of the nuclear spin correlations within rotating and precessing molecules. These effects involve virtually all J levels, particularly the higher ones, and they occur in the *absence* of external fields. Because a semiclassical approach provides a much clearer picture of rotation and precession, it is easier to see how localized correlations come about and what combinations of Pauli-allowed spin–rotation states are stationary.

Furthermore, these developments do not appear to be at all specialized when viewed in the light of future possibilities. The quantum optics research of Bordé, J. Hall, and others is heading toward highly nonlinear spectroscopies in which systems will be prepared in states that are highly nonstationary. The developments described in PHYSICS TODAY are well suited for visualizing the dynamics of many different types of subtle and complex molecular motions.

That Bunker says the presentation is in the manner of "Madison Avenue" is surprising, given that Bunker titled one of his publications "Practically everything you ought to know about molecular symmetry." Contrary to the implications of his title, we believe there will be many new things to know about molecular symmetry and dynamics, and that the results described in PHYSICS TODAY represent just a few of the verifiable examples. When a research group has conclusively demonstrated some new effect, they should be encouraged to publicize them. Atomic, molecular and optical physics has as many new ideas, results and applications as other subfields, but it has not been as skillful in presenting them to a more general audience. The field will not grow if its members are content to just sit on their Hamiltonians and pretend that there is nothing new.

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ERIC J. HELLER COMMENTS: It seems that many of the physicists in this country doing theoretical work on atomic and molecular theory are concerned about the level of support for the field, the number of students going into it, and the perception of the field by other physicists and other scientists. It is therefore with some sadness that I read Philip Bunker's letter regarding the Harter–Patterson rotational clustering theory. I do not think anyone can deny that Harter and Patterson have a unique point of view and have made much progress on an important problem. It is also natural and appropriate that Bunker should want to point out the progress of the past 20 years, made by many people, in the

continued on page 124

continued from page 15

understanding of vibration–rotation spectra of polyatomic molecules. What is sad is that he chose to do so by attempting to belittle the Harter–Patterson work. There is no doubt that the work of Hougen, Watson, and others has been equally deserving of PHYSICS TODAY coverage in years past. Fault for this does not lie in a July 1984 "Search and discovery" article, but rather in a collective failure of physicists in the field to generate the enthusiasm necessary for this kind of coverage. Harter and Patterson present a new, dynamic point of view, both figuratively and literally. If it attracts a public following, then so much the better for the rest of us. Instead of bickering, we should be bootstrapping ourselves into higher prominence in physics, with the attendant increase in funding and student interest. Let us hope that Bunker's letter is just an isolated example, and not the beginning of a trend.

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"RECENTLY LUDWIG MIZZELDORP CAME UP WITH SOME STARTLING DISCOVERIES IN THE FIELD OF SUB-ATOMIC PARTICLES. I'D LIKE TO SING YOU SOME OF HIS FORMULAS."

Physics and the military

It is difficult to believe that anyone as smart as Charles Schwartz could be so oblivious to the obvious. In his guest comment for October (page 9), he devotes several pages to illustrating how physicists either wittingly or unwittingly contribute to the military security of the United States, the point of it all being that it is wrong, wrong, wrong. But it is Schwartz who is wrong.

The obvious facts are that the Soviet Union is a totalitarian dictatorship bent on world domination through the spread of its system to all corners of the globe; that the Soviet Union has been thwarted in its schemes by the military power of its chief adversary; that if the Soviet Union were truly interested in a verifiable control of weaponry, it would agree to on-site inspections; and that if all the physicists in the United States followed Schwartz's suggestions to weaken our military preparedness, there would be unbounded glee in the Kremlin.

Schwartz bemoans the risks of stockpiling nuclear weapons, but the fact is that until nuclear weapons were stockpiled, wars were wreaking havoc on this planet with increasing destruction and frequency. It seems very likely, on the basis of experience, that had only conventional weapons been available, a third world war, pitting the democracies against Russia and her satellites, would already have battered the earth.

No one likes living with potential annihilation. But I prefer that risk to the certainty of conventional war or to life under the Soviet system. I especially prefer that risk in light of the fact that the nuclear deterrent has given us peace and freedom during 40 years of the most dangerous of provocations.

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Degeneracy in perturbation

The insidiousness of degenerates was recently brought home to me subsequent to preparing a lecture on time-independent perturbation theory for my quantum course. The subject was the case of degenerate levels. For some time, I had believed that the first-order corrections to the "correct" zero-order degenerate eigenkets were orthogonal to the subspace S spanned by these kets. When I tried to prove this, however, I soon discovered that such orthogonality was generally incompatible with the second-order equations which, somewhat to my surprise, together with normalization conditions, determine the projections of the first-order corrections on S. A short calculation using the second-order equations gives, in fact:

$$|E_n{}^{(1)}\rangle = \sum_{s>g} \frac{V_{sn}|E_s\rangle}{E_n - E_s} + \sum_{\substack{m<g \\ m\neq n}} \frac{V_{mt}V_{tn}|E_m\rangle}{(E_n - E_t)(V_{nn} - V_{mm})}.$$

Here, $|E_n{}^{(1)}\rangle$ is the first-order correction to the correct zero-order ket $|E_n\rangle$, assumed to be degenerate in zero-order with the kets $|E_m\rangle$, $m = 1, \ldots g$. The latter are all assumed to be the correct zero-order kets that is, they are chosen so that the off-diagonal elements $\langle E_m|V|E_p\rangle \equiv V_{mp}$, $m \neq p$ vanish for m and p less than g. The second term on the right-hand side is, of course, the projection of $|E_n{}^{(1)}\rangle$ on S and was quite unexpected.

Puzzled as to the source of my mistaken belief, I then reviewed the quantum theory books close at hand and found that most of the authors who explicitly addressed this point erroneously asserted or implied orthogonality (references 1–10). I found the correct treatment in only a few books (references 11–14). When our students submit papers to us which contain identical errors, we often suspect the absence of independent thought. Should the same principle also apply to the authors of physics texts?

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