

LEP Tunnel Comes Full Circle



The excavation of the 27-kilometer-circumference LEP tunnel was completed on 8 February with a final explosion detonated under the Jura mountains near Geneva. This picture, taken a few days earlier in front of the drilling head in a nearby section of the tunnel, shows LEP project leader Emilio Picasso (yellow coat), flanked by his assistant Günther Plass (right, black jacket) and Henri Laporte (left), head of civil engineering for this gargantuan electron-positron storage-ring collider.

From its injector complex at CERN, the LEP ring makes its way under Swiss and French countryside and mountains. The schedule calls for the beam pipe to be sealed and evacuated on 14 July 1989—the 200th anniversary of the storming of the Bastille. Once the ring is evacuated, it will store countercirculating beams of 50-GeV electrons and positrons. Useful electron-positron collision rates at the four intersection points are expected to be available to experimenters less than four months thereafter. No great difficulty is foreseen, because LEP, unlike the recently completed Stanford Linear Collider, is basically a conventional storage ring.

the correlation term in the Hamiltonian. One performs a variational calculation to find the superposition state of minimum energy in this expanded Hilbert space. Before the advent of very powerful computers in the last decade, such a computational program would have been impractical. Even with access to a Cray X-MP, Froese Fischer was forced by the large number of configuration states involved to make significant simplifying assumptions. She did not, for example, include correlations between the valence electrons of calcium and the 18 inner electrons of its argon-like core.

Froese Fischer undertook to calculate the energy difference between the $4s^2$ (1S) ground state of Ca^0 and the $4s^2 4p$ (2P) state of Ca^- , to see which was lower. Lagowski and Vosko had pointed her toward the $4s^2 4p$ state of the negative ion rather than the more obvious $3d 4s^2$ configuration because it was known from earlier experimental work of Lineberger and his coworkers that the stable negative ion of scandium has its extra electron in the $4p$ orbital rather than the $3d$ orbital one

might have expected. Lagowski and Vosko had been unable to explain this puzzling state of affairs with a conventional single-particle Hartree-Fock calculation. Therefore Froese Fischer began with a multiconfigurational Hartree-Fock calculation for Sc^- . For the negative scandium ion, unlike Ca^- , the experimental situation was known. "But when I saw how drastically the correlation energy for Sc^- was lowered in the multiconfigurational Hartree-Fock calculation when I switched the extra electron from $3d$ to $4p$, I suddenly realized that this might be what's happening in calcium—why Pegg hadn't seen Ca^- fall apart. In conventional independent-particle Hartree-Fock calculations that don't include correlations, one could never get a bound $4p$ electron in a scandium or calcium ion."

Before Froese Fischer introduces $4d$, $5s$, and $5p$ components into her multiconfigurational calcium calculation, she cannot get a stable Ca^- ion. The $4s^2$ ground state of neutral calcium remains 0.2 eV below the $4s^2 4p$ state of Ca^- —an energy difference of

one part in 10^5 . When she introduces the higher-orbital contributions, the sign of this tiny energy difference reverses. But not until she introduces contributions up to $6p$ does she get a binding energy comparable to what Pegg and company later found in the laboratory. In fact, with these $n = 5$ and 6 contributions, the calculated electron affinity overshoots to 0.056 eV until relativistic corrections bring it back down to 0.045 eV, in excellent agreement with the experimental result that was soon to come.

To complement Froese Fischer's multiconfigurational Hartree-Fock calculations, Lagowski and Vosko carried out density-functional-theory calculations for Ca^- and Sc^- . The density-functional approach treats correlations at the conventional single-particle Hartree-Fock level by including an effective "correlation potential" term in the Hamiltonian. It is known to be a less accurate computational technique, but its greater simplicity yields useful qualitative insights into the unexpected configuration of the stable Ca^- state. Lagowski and Vosko conclude from this calculation that the extra electron goes into $4p$ rather than $3d$ essentially because the $3d$ orbital has a greater wavefunction overlap with the electron core, and hence a larger classical Coulomb repulsion energy.

What about the other alkaline earths? It looks as if much the same thing should happen for strontium (neutral ground state $5s^2$). The textbook cliché about the alkaline earths is certainly dead. But the lightest and heaviest group IIA elements are somewhat different. Beryllium ($2s^2$) and magnesium ($3s^2$) do not possess the vacant d -orbital state just below the outer shell that appears to play a crucial role in binding the extra p -orbital electron. At the heavy end of group IIA, barium ($6s^2$) and radium ($7s^2$) have nearby vacant ($n - 2$) f orbitals that make it difficult to guess whether they could bind an extra electron. And we have seen how good qualitative guesses are in the absence of calculations that take adequate account of electron correlations.

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References

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