HMD Development: An Event Generator for Simulation of Heavy Ion Transport

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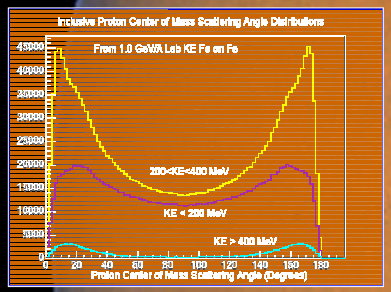
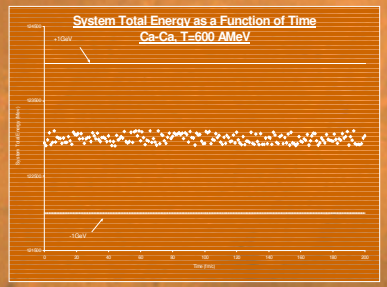
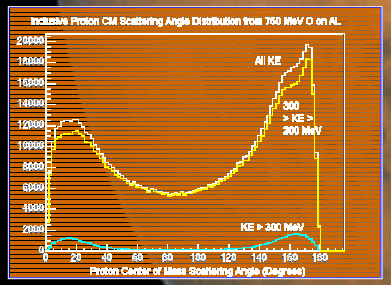
Introduction

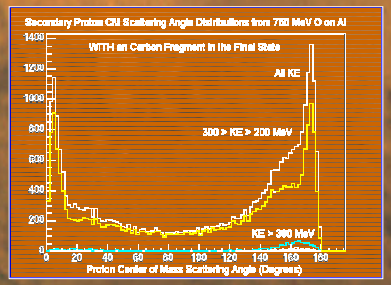
Simulation of the nuclear reactions induced by heavy ions impinging on material represents a long-standing difficulty for calculations associated with radiation exposure in the space environment. Common approaches to this problem are difficult to implement as event generators for simulation due to the structure of the formalism. Typical model results are either quasi-analytic expressions for total cross section as a function of CM energy, or simulations in which nuclei are expressed as collections of non-interacting nucleons, removing any coherence or fragment formation information.

A promising simulation theory for this type of problem presents itself in the so-called Quantum Molecular Dynamics (QMD), in which a first-principles approach is taken with regard to system description with no a priori need for scaling of results or in-model fitting of experimental data. As is seen with previous attempts to implement this approach to ion scattering, the major difficulty in making use of these QMD theories is the inclusion of particle interactions in a covariant manner. To address this difficulty, we turn to the constrained Hamiltonian formalism of Dirac as developed by Todorov, Komar, Maruyama, and others. The resulting model we dub HMD, or Hamiltonian Molecular Dynamics. Here we present a brief description of the fully covariant theoretical development, as well as the development status of the resulting model code.









Method

The MHD model is based on the concept of the constrained Hamiltonian as introduced by Dirac, and developed by Todorov and Komar. Effective nucleon-nucleon potentials are given in a non-relativistic form (e.g. as a function of 3-distance). Clearly the challenge then is to cast nucleon (and thus nuclear) equations of motion which are nevertheless manifestly covariant. In moving from a Wigner-picture 6-N dimensional quasi-phase space to Minkowski space, we see the number of degrees of freedom obviously increase by 2N. Thus, 2N equations of constraint allow us to uniquely define the world-lines for each particle in the system.

Potentials are included by making the philosophical approximation that the effect of the potentials on system trajectory is to alter the transverse momentum distributions, so that the argument of the potential functional is transformed to the transverse 4-distance, making the potentials by definition Poincaré scalars. Working according to the constrained Hamiltonian formalism, the Hamiltonian is written as a linear combination of the (scalar) constraint equations, the coefficients being elements from the inverse of the Poisson matrix. We believe that the energy conservation issues realized by previous authors are overcome via a tedious, but necessary individual calculation and combination of single-particle Hamiltonians and correlation (potentials and Hilbert coherence) energies. This has been shown for a limited range of systems, and validation of this contention is currently ongoing.

In its current form, this model makes use of the free-particle nucleon-nucleon elastic cross sections to describe successive particle collisions, with no inclusion of inelastic channel probabilities. We recognize that this is insufficient for a full description of the system, both in terms of the inclusion of inelastically produced products, and the alteration to some form of in-medium cross section set. This addition is necessarily going to be made, and the current approximation has been made not as a philosophical decision about the system under study, but rather as a first-order approximation made for simplicity as the theory is developed and the code validated.

Because of the reliance of this method on semi-classical Hamilton-Jacobi theory, Pauli blocking, fragment coalescence, and any final state interactions are included formally rather than being a natural consequence of the central theory. Pauli blocking is included such that a particle cannot scatter back into a state with momentum below the Fermi level in its original nucleus. Coalescence is achieved through an again tedious, but necessary calculation of combinatorial possibilities based on proximity with regard to spatial coordinate (4-vector) and momentum, effectively working towards a minimization of "coalescence volume" in Minkowski space. Final state interactions are included by allowing further collisions and interactions between any after the initial set of reactions characteristic of the two nuclei passing through the overlap or "fireball" region, including interactions between product fragments.

Status and Discussion

This model is not complete, but is currently in an advanced stage of development. Particle propagation, collision, and coalescence models exist, but as separate pieces of code still needing to be integrated into a useable package. Shown here are preliminary results showing the level of energy conservation achieved, as well as examples of the manifestation of Hilbert state coherences in scattering data already achieved by earlier implementations of the same theory. Clearly it is possible to see some of the effects of entanglement on the final observable states. For simulating the structure of radiation fields in a realistic way, this is a very desirable result, in that one can observe a level of predictive capability and understanding of the environment surpassing methods built on the need to express nuclei as a collection of non-interacting particles, or on methods resulting in an estimate of total yield.

We expect to have a fully operational scattering event generator ready for data confrontation by October '04. At that point the limiting factor in the validation effort will be the availability, and in fact the existence of anything approaching exclusive data sets. Of paramount importance in our opinion is the need for any future attempt to make these measurements to include momentum distributions of neutrals in addition to the charged particle yields, so that simulations can be judged against raw performance without the need to integrate the fundamental 4-differential cross sections.

References

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HMD Event Generator

(Hamiltonian Molecular Dynamics)

- Goal: Develop an event generator for heavy ion collision simulation
  - Built from pure theory – for extrapolation to regions of little or no data
- Quantum Molecular Dynamics Framework
  - Pauli blocking
  - State correlations – Exclusive events
  - Fully covariant system description
  - Fragment formation / coalescence
- First integreation into FLUKA hopefully Fall ’04 release (or next)