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Monte Carlo evaluation of the semiclassical multi-step direct reaction series

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Abstract. We show how the multi-step direct reaction series can be evaluated using Monte Carlo methods. Nucleon-nucleon collisions occur according to the random selection of a nucleon's attenuation factor along its classical trajectory. The particles and hole excited in a collision are selected from a local Fermi distribution. We assume that the particles continue to propagate and possibly collide again before leaving the nucleus. We assume that holes collide in place, to possibly produce other particles and holes.

1 Introduction

Nucleon-induced pre-equilibrium reactions are recognized to consist almost exclusively of direct reactions in which incident nucleons induce excitations over a wide range of energy in the target nucleus. At low energies, one step reactions dominate. As the incident energy increases, multi-step reactions become important too. Although quantum mechanical models of these reactions were introduced long ago, [1–3] their computational difficulty has limited their application to calculations including at most two steps,[2, 4–7] in most cases, and four steps in a particular simplified model.[8]

Some twenty years ago, Kawai and collaborators used the Wigner transform to rewrite the multi-step direct reaction series directly as a sum of cross sections rather than squared amplitudes. [9–13] Such a transformation can be performed exactly, if one makes the usual assumption that amplitudes involving different numbers of collisions are incoherent. They further simplified the expressions for the cross sections by rewriting the incoming and outgoing waves, as well as intermediate propagators, in terms of classical trajectories and quantum absorption factors. Calculations have been extended up to third order and provide promising results when compared to experimental data. [14, 15] However, the calculations continue to be computationally demanding.

We show how the semiclassical multi-step series can be evaluated using Monte Carlo methods. Nucleon-nucleon collisions occur according to the random selection of a nucleon's attenuation factor along its classical trajectory. In a more precise model, the particle and hole excited in a collision would be selected randomly from a sum of Wigner densities. For the moment, we plan to select them from a local Fermi distribution, which furnishes distributions similar to those of Kikuchi and Kawai. [16] We assume that the continuum particles produced

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continue to propagate and possibly collide again before leaving the nucleus. We assume that holes collide in place, to possibly produce other particles and holes. The resulting model has a striking resemblance to the DDHMS model of Blann and Chadwick. [17, 18] However, it goes beyond that model by including the dependence on impact parameter and quantum absorption and transmission factors, as well as permitting the eventual inclusion of curved trajectories.

2 The quantum multi-step direct reaction series

The usual development of the quantum multi-step (nucleon-induced) direct reaction series begins by assuming that the space of relevant states can be separated into a sequence of bound states and a sequence of one-particle continuum states distinguished by the number of particles and holes and accessible through a momentum and energy conserving two-body interaction. [1–3] The sequences can be represented as in Fig. 1 where $P_{1,0}$ represents the initial continuum configuration of the projectile nucleon incident on a target in its ground state, while $P_{2,1}$ and $Q_{2,1}$ represent the configurations in which the projectile nucleon is in the continuum or a bound state, respectively, while a particle-hole pair has been created in the target nucleus. The configurations with more particle-hole pairs can be reached through further collisions, as denoted by the arrows in the figures.

The multistep direct Hamiltonian consists of an optical Hamiltonian describing the propagation of the projectile, an internal Hamiltonian describing target excitations and an interaction coupling the two,

$$H = H^{opt} + H^{int} + V. \tag{1}$$

The optical potential takes into account the loss of flux due to target excitation as well as other processes not included explicitly in the multi-step Hamiltonian. The internal Hamiltonian furnishes a set of single-particle states of the target, $H^{int}\phi_a = \epsilon_a\phi_a$, which, at the one-particle-one-hole level, can be combined to furnish transition densities to excited states μ of the target. For example, using a Tamm-Dancoff or random phase approximation, or even simple particle-hole excitations, with the coefficient for the nucleon in state a to be excited to state b having the coefficient X^{μ}_{ab},

$$\rho_{\mu}\left(\vec{r_0}\right) = \sum_{a,b} X^{\mu}_{ab}\phi^{\dagger}_{b}\left(\vec{r_0}\right)\phi_a\left(\vec{r_0}\right). \tag{2}$$

The interaction coupling the projectile motion to target excitation is a sum over a nucleon-nucleon interaction over the possible nuclear excitations,

$$V\left(\vec{r}\right) = \sum_{\mu} V_{\mu}\left(\vec{r}\right) = \int d^3r\, v\left(\vec{r}-\vec{r}_0\right)\sum_{\mu}\rho_{\mu}\left(\vec{r}_0\right). \tag{3}$$

The contribution to the wave function of a particular one-step excitation μ would take the form,

$$\left|\Psi^{(+)}_{\nu}\right\rangle = G^{+}_{\nu}(E)V_{\mu}\left|\Psi^{(+)}_{0}\right\rangle, \tag{4}$$

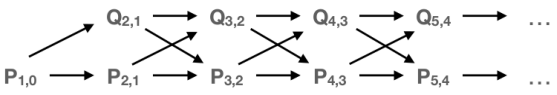

Figure 1. Schematic diagram of multi-step direct/compound reaction series.

while that for a two step excitation of $\mu + \nu$ could be written in terms of the two one-step processes as

$$\left|\Psi^{(+)}_{\mu+\nu}\right\rangle = G^{+}_{\mu+\nu}(E)\left(V_\mu \left|\Psi^{(+)}_{\nu}\right\rangle + V_\nu \left|\Psi^{(+)}_{\mu}\right\rangle\right). \tag{5}$$

The full wave-function includes the contributions of all one-step and two-step excitations as well as higher order ones,

$$\left|\Psi^{(+)}\right\rangle = \left|\psi^{(+)}_0\right\rangle \delta_{\mu,0} + \sum_\mu G^{+}_{\mu}(E) V_\mu \left|\psi^{(+)}_0\right\rangle + \sum_{\mu,\nu} G^{+}_{\mu+\nu}(E) V_\mu G^{+}_{\nu}(E) V_\nu \left|\psi^{(+)}_0\right\rangle + \ldots. \tag{6}$$

The T-matrix for populating a given asymptotic state m is given by its overlap with the full wave-function, which we can write to third order in the coupling as

$$\begin{aligned} T_{m0} \;=\; & \sum_\mu \left\langle \psi^{(-)}_m \right| V_\mu \left|\psi^{(+)}_0\right\rangle + \sum_{\mu,\nu} \left\langle \psi^{(-)}_\alpha \right| V_\mu G^{+}_{\nu}(E) V_\nu \left|\psi^{(+)}_0\right\rangle \\ & + \sum_{\mu,\nu,\kappa} \left\langle \psi^{(-)}_\alpha \right| V_\mu G^{+}_{\nu+\kappa}(E) V_\nu G^{+}_{\kappa}(E) V_\kappa \left|\psi^{(+)}_0\right\rangle + \ldots. \end{aligned} \tag{7}$$

Up to a phase space factor, the cross section can be written as the magnitude squared of the T-matrix element. To reduce this to a sum of squares, we assume that the contributions of the different excitation modes to a given final state m are incoherent, so that cross terms in the sum vanish.[1–3] We can then write the cross sections as a sum over independent one-step, two-step, and higher order cross sections,

$$\begin{aligned} \frac{d^2\sigma}{dE_m d\Omega_m} \;=\; & \overline{\left|\sum_\mu \left\langle \psi^{(-)}_m \right| V_\mu \left|\psi^{(+)}_0\right\rangle\right|^2} + \overline{\left|\sum_{\mu,\nu} \left\langle \psi^{(-)}_m \right| V_\mu G^{+}_{\nu}(E) V_\nu \left|\psi^{(+)}_0\right\rangle\right|^2} \\ & + \overline{\left|\sum_{\mu,\nu,\kappa} \left\langle \psi^{(-)}_m \right| V_\mu G^{+}_{\nu+\kappa}(E) V_\nu G^{+}_{\kappa}(E) V_\kappa \left|\psi^{(+)}_0\right\rangle\right|^2} + \ldots. \end{aligned} \tag{8}$$

Although transition densities for multi-step processes are usually expressed in terms of unoccupied bound-particle states, there are actually very few unoccupied bound states in a typical nucleus. Practical transition functions must also take into account excitations to the continuum, that is, knockout reactions, which extend the transition function as

$$\rho_\mu(\vec{r_0}) \to \sum_{a,b} X^{\mu}_{ab} \phi^{\dagger}_b(\vec{r_0})\, \phi_a(\vec{r_0}) + \sum_a \int d^3k_b\, X^{\mu}_{ab} \psi^{\dagger}_{\vec{k}_b}(\vec{r_0})\, \phi_a(\vec{r_0}). \tag{9}$$

However, as the emphasis of the multi-step direct series is on the leading projectile particle, the continuum excitations of the target are usually approximated as bound ones.

3 An alternative development of the multi-step direct reaction series

Here we analyze the Wigner-transform of the multi-step direct reaction series, in preparation for its evaluation using Monte Carlo methods.

3.1 The Wigner transform

The Wigner transform[19] converts a wave function into a coordinate- and momentum-dependent quasi-probability phase-space distribution as

$$\Psi\left(\vec{\kappa},\vec{R}\right)=\int d^3s\, e^{-i\vec{\kappa}\cdot\vec{s}}\psi\left(\vec{R}+\vec{s}/2\right)\psi^\dagger\left(\vec{R}-\vec{s}/2\right). \tag{10}$$

Although other transformations of a wave function to a phase-space distribution are possible, the Wigner transform has the special property of furnishing the correct coordinate probability distribution, when the momentum variable is integrated,

$$\frac{1}{(2\pi)^3}\int d^3\kappa\,\Psi\left(\vec{\kappa},\vec{R}\right)=\psi\left(\vec{R}\right)\psi^\dagger\left(\vec{R}\right), \tag{11}$$

and of furnishing the correct momentum distribution, when the coordinate variable is integrated,

$$\int d^3R\,\Psi\left(\vec{\kappa},\vec{R}\right)=\int d^3r\,d^3r'\,e^{-i\vec{\kappa}\cdot\vec{r}}\psi\left(\vec{r}\right)\,e^{i\vec{\kappa}\cdot\vec{r}'}\psi^\dagger\left(\vec{r}'\right)=\psi\left(\vec{\kappa}\right)\,\psi^\dagger\left(\vec{\kappa}\right). \tag{12}$$

3.2 The one-step cross section

The squared one-step direct matrix element can be written in terms of Wigner transformed wave functions and transition densities[9–13] and a Fourier transformed nucleon-nucleon interaction V as

$$\begin{aligned}\left|\left\langle\psi_m^{(-)}\left|V_\mu\right|\psi_0^{(+)}\right\rangle\right|^2 &= \frac{1}{(2\pi)^9}\int d^3Rd^3\kappa_f d^3\kappa_i\Psi^{(-)\dagger}_{\vec{k}_m}\left(\vec{\kappa}_f,\vec{R}\right)\Psi^{(+)}_{\vec{k}_0}\left(\vec{\kappa}_i,\vec{R}\right)\\ &\times\int d^3R_0\,d^3p\,d^3Q\,e^{i\vec{p}\cdot\left(\vec{R}-\vec{R}_0\right)}K_\mu\left(\vec{Q},\vec{R}_0\right)\\ &\times\delta\left(\vec{\kappa}_i-\vec{\kappa}_f+\vec{Q}\right)V\left(\vec{Q}+\vec{p}/2\right)V^\dagger\left(\vec{Q}-\vec{p}/2\right).\end{aligned} \tag{13}$$

The transformed expression for the matrix element makes no approximation. However, as the nucleon-nucleon in interaction $V\left(\vec{r}\right)$ is of short range, we expect its Fourier transform $V\left(\vec{q}\right)$ to be relatively smooth, justifying the approximation,

$$V\left(\vec{Q}+\vec{p}/2\right)V^\dagger\left(\vec{Q}-\vec{p}/2\right)\approx\left|V\left(\vec{Q}\right)\right|^2. \tag{14}$$

This approximation reduces the integral defining the matrix element to an integral over the initial and final Wigner momenta and over a single coordinate,

$$\begin{aligned}\left|\left\langle\psi_m^{(-)}\left|V_\mu\right|\psi_0^{(+)}\right\rangle\right|^2 &\approx \frac{1}{(2\pi)^6}\int d^3R\,d^3\kappa_f\,d^3\kappa_i\,\Psi^{(-)\dagger}_{\vec{k}_m}\left(\vec{\kappa}_f,\vec{R}\right)\Psi^{(+)}_{\vec{k}_0}\left(\vec{\kappa}_i,\vec{R}\right)\\ &\times\int d^3Q\,K_\mu\left(\vec{Q},\vec{R}\right)\left|V\left(\vec{Q}\right)\right|^2\delta\left(\vec{\kappa}_i-\vec{\kappa}_f+\vec{Q}\right).\end{aligned} \tag{15}$$

Taking into account the statistical incoherence of the different contributions to the one-step cross section, we can write[20]

$$\sum_{\mu\in\Delta E}K_\mu\left(\vec{R},\vec{Q}\right)\approx\sum_{\mu\in\Delta E}\sum_{a,b}\left|X^\mu_{ab}\right|^2\int d\kappa_a^3d\kappa_b^3\,\Phi_b^\dagger\left(\vec{R},\vec{\kappa}_b\right)\Phi_a\left(\vec{R},\vec{\kappa}_a\right)\times\delta\left(\vec{\kappa}_a-\vec{\kappa}_b-\vec{Q}\right).$$

In order to evaluate this expression, we must first obtain expressions for the wave fiunctions and transitions densities that enter it.

3.3 The eikonal approximation to the scattering states

At this stage in the development of the model, we prefer to develop the wave functions in an extended eikonal approximation. In this case, we write the incoming scattering wave functions as

$$\psi^{(+)}_{\vec{k}}\left(\vec{r}\right) = \exp\left[i\int_{-\infty}^{z}\kappa\left(z',\vec{b}\right)dz' - \frac{1}{2}\ln\left(\kappa\left(z,\vec{b}\right)\right)\right], \tag{16}$$

where the complex wave number is written in terms of the complex optical potential as

$$\kappa\left(\vec{r}\right) = \sqrt{k^2 - \frac{2\mu}{\hbar^2}\left(V\left(\vec{r}\right) - iW\left(\vec{r}\right)\right)} \tag{17}$$

with the coordinate $z = \hat{k}\cdot\vec{r}$ along the direction of propagation and impact parameter $\vec{b} = \vec{r} - z\hat{k}$. Substituting into Eq. (11) and expanding the terms in the exponential to first order in the separation vector $\vec{s}$, the incoming Wigner distribution can be approximated as the product of a trajectory term and a term that takes into account the attenuation of the flux as well as its variation with velocity,

$$\Psi^{(+)}_{\vec{k}}\left(\vec{\kappa},\vec{R}\right) \approx (2\pi)^3\,\delta\left(\vec{\kappa} - \vec{\kappa}_+\left(\vec{R},\vec{k}\right)\right)\left|\chi^{(+)}_{\vec{k}}\left(\vec{R}\right)\right|^2, \tag{18}$$

where the flux attenuation is determined by the imaginary part of the trajectory integral,

$$\left|\chi^{(+)}_{\vec{k}}\left(\vec{R}\right)\right|^2 = \frac{k}{\left|\kappa(Z,\vec{B})\right|}\exp\left[-2\int_{-\infty}^{Z}\mathrm{Im}\,\kappa(z',\vec{B})dz'\right]. \tag{19}$$

In the absence of absorption, the inverse variation with velocity of the Wigner distribution assures local density conservation.

The momentum trajectory is given by the integral of the variation of the momentum,

$$\vec{\kappa}_+\left(\vec{R},\vec{k}\right) = \vec{k} + \int_{-\infty}^{Z}\mathrm{Re}\vec{\nabla}\kappa\left(z',\vec{B}\right)dz' = \vec{k} - \frac{\mu}{\hbar^2}\int_{-\infty}^{Z}\mathrm{Re}\frac{1}{\kappa\left(z',\vec{B}\right)}\vec{\nabla}U\left(z',\vec{B}\right)dz'. \tag{20}$$

We observe in the last line that the integral can be associated with the variation of the momentum given by Newton's Second Law, when we recognize the relation, $\mu dz'/\hbar\kappa \approx dt$.

When the incoming/outgoing Wigner distributions are substituted in the one-step matrix element squared, the latter reduces to

$$\begin{aligned}\left|\left\langle\psi^{(-)}_m\left|V_\mu\right|\psi^{(+)}_0\right\rangle\right|^2 \approx & \int d^3R\,\Psi^{(-)\dagger}_{\vec{k}_m}\left(\vec{\kappa}_-\left(\vec{R},\vec{k}_m\right),\vec{R}\right)\Psi^{(+)}_{\vec{k}_0}\left(\vec{\kappa}_+\left(\vec{R},\vec{k}_0\right),\vec{R}\right) \\ & \times\int d^3Q\,K_\mu\left(\vec{Q},\vec{R}\right)\left|V\left(\vec{Q}\right)\right|^2\delta\left(\vec{\kappa}_+\left(\vec{R},\vec{k}_0\right) - \vec{\kappa}_-\left(\vec{R},\vec{k}_m\right) + \vec{Q}\right).\end{aligned} \tag{21}$$

Thus the eikonal approximation to the incoming/outgoing Wigner wave distributions reduces the one-step matrix element to a single integral over the coordinate $\vec{R}$.

3.4 Transition functions and bound state wave functions

Another important quantity in the one-step matrix element is the transition function. Consider here an inclusive transition function, obtained by summing over all excitations μ. We approximate this as

$$\begin{aligned}\sum_\mu\rho_\mu\left(\vec{r}\right)\rho^\dagger_\mu\left(\vec{r}'\right) \rightarrow \sum_\mu K_\mu\left(\vec{R},\vec{Q}\right) \rightarrow & \int d\kappa_a^3 d\kappa_b^3\,\delta\left(\vec{\kappa}_a - \vec{\kappa}_b - \vec{Q}\right) \\ & \times\sum_{b\in nocc}\Phi^\dagger_b\left(\vec{R},\vec{\kappa}_b\right)\sum_{a\in occ}\Phi_a\left(\vec{R},\vec{\kappa}_a\right),\end{aligned} \tag{22}$$

where the $\Phi_i\left(\vec{R},\vec{\kappa}_i\right)$ are the Wigner distributions corresponding to the single-particle states of the target nucleus.

Martorell and Moya de Guerra[21] have shown that the sum of the Wigner distributions corresponding to the $(K+1)(K+2)/2$ single-particle states of energy $\hbar\omega(K+3/2)$ of the harmonic oscillator (HO) shell with principal quantum number K, $K = 0, 1, 2, \ldots$ can be written in terms of the associated Laguerre polinomial $L_K^2(h)$ as

$$\sum_{a\in K}\Phi_a\left(\vec{R},\vec{P}\right) = (-1)^K\, 8\, e^{-h/2}\, L_K^2(h)\,, \tag{23}$$

where h is related to the classical HO Hamiltonian as

$$h/2 = P^2b^2 + R^2/b^2 \tag{24}$$

with $b \approx A^{1/6}$ fm being the quantum HO length, A being the target mass number. If we assume the nucleus to have two protons and two neutrons in each of the single particle states up to the principal quantum number N, we have

$$A = 4\sum_{K=0}^{N}\frac{1}{2}(K+1)(K+2) = \frac{2}{3}(N+1)(N+2)(N+3)\,. \tag{25}$$

The marginal distributions $\rho(R)$ and $\rho(P)$ corresponding to the Wigner HO distributions summed over all states up to principal quantum number N are the corresponding quantum HO densities in coordinate and momentum space, respectively. We have analyzed these for $N = 2$, 4, 6, and 8. In Fig.2(a-b), we display the momentum distributions $\rho_N(p)$ together with the Fermi function,

$$\rho_F(x) = 1/\left(1+\exp\left[(x-x_F)/a_F\right]\right), \tag{26}$$

where we also compare the phase-space weighted densities $p^2\rho(p)$ with the weighted Fermi function, $p^2\rho_F(p)$. The momentum distributions are all surprisingly similar. Although these are much greater than one in the low momentum region, the weight factor suppresses the difference, so that the weighted distributions are in fact quite similar to the weighted Fermi function. A fit of the weighted Fermi function to the weighted momentum distributions furnishes

$$p_F = 1.09\ \text{fm}^{-1} \quad \text{and} \quad a_F = 0.132\ \text{fm}^{-1}. \tag{27}$$

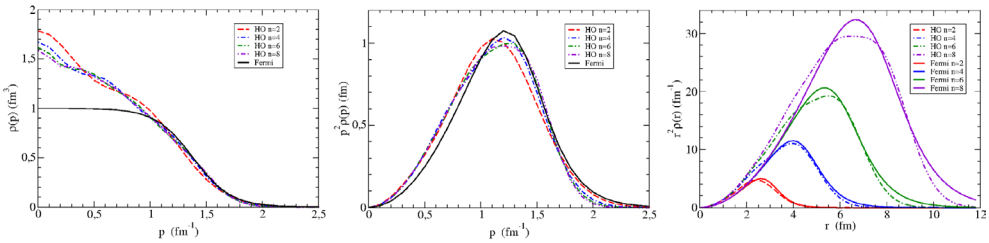

Figure 2. (a-b) HO marginal momentum distributions and phase-space weighted distributions are compared to a Fermi distribution and its phase-space weighted counterpart. (c) Phase space weighted HO marginal coordinate distributions are compared to the corresponding phase space weighted Fermi distributions.

In Fig.2(c), we show the corresponding weights HO coordinate densities, which grow in magnitude and extension with the quantum number N. After analyzing the dependence on the oscillator length b of the quantity h determining the momentum and coordinate distributions, it is not surprising that we can fit the coordinate densities with (26) where

$$r_F = r_0 A^{1/3} \text{ with } r_0 = 1.09 \text{ fm, and } a_F = a_0 A^{1/3} \text{ with } a_0 = 0.132 \text{ fm.}$$

Although it should come as no surprise, we have shown that the marginal HO momentum and coordinate distributions take forms similar to those we would expect of nuclear momentum and coordinate densities. The Wigner HO distributions that enter the transformed transition density are not the marginal ones however, but the complete ones. As these are not positive for all values of the coordinate and momentum, further study will be necessary to use these in the Monte Carlo procedure we intend to implement.

4 A Monte Carlo method

We can extend the development to the two-step and higher order excitation matrix elements. However, the Wigner transformed multi-step direct series is just as complicated to evaluate as the original one. It also continues to suffer from the deficiency of the original series in that it treats the incident particle differently from other particles excited to the continuum in the collision process. Yet, the Wigner transformed series has the potential of being manipulated into a form in which its contributions are always positive, making it amenable to a Monte Carlo type of evaluation.

As the principal Monte Carlo selector for nucleon-nucleon collisions, we plan to use the attenuation factor of the Wigner transformed wave function, as such collisions are the principal source of optical model absorption. Nucleon-nucleon collisions can then be evaluated using Monte Carlo selection according to the phase space available from the transition density. For the moment, we plan to select from a local Fermi distribution, which furnishes particle and hole distributions similar to those of Kikuchi and Kawai. [16] To complete the evaluation, all particles in the continuum should be submitted to such an evaluation process.

A complete algorithm for one event of the Monte Carlo evaluation would consist of the following steps:

0) Initiate an event by randomly selecting an impact parameter for the projectile.

1) Randomly choose a particle from the stack of particles in the continuum. (Initially, the projectile is the only particle in the stack.)

2) Propagate the particle on a straight line in accord with its initial momentum, accumulating the change in its momentum and its attenuation until the latter reaches a prescribed value selected randomly.

a) If the prescribed value is not reached, the particle is emitted with a momentum that takes into account its deflection from the initial direction while propagating to infinity.

b) If the prescribed value of the attenuation is reached, initiate a collision at the location reached using a momentum that takes into account the deflection accumulated. Choose the two final particles and the hole according to the phase space available for the collision in the transition function and place any continuum particles in the particle stack. If the hole has enough energy to form a continuum particle in a subsequent collision, start a new collision with it and place any produced continuum particles in the stack. Continue until no hole is produced with sufficient energy to produce a continuum particle. Bound particles and low-energy holes are dumped into the compound nucleus.

c) Return to 1) until there are no more continuum particles in the stack.

3) Proceed to evaluation of emission from the remaining compound nucleus.

4) Initiate a new event.

Such a procedure is similar to that used in many Monte Carlo cascade codes as well as in Blann's hybrid Monte Carlo pre-equilibrium model.[17, 18] Basing the method on the Wigner transformed multi-step direct series furnishes a well-defined basis that should make possible systematic improvement in the future.

Acknowledgments

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