IONIZATION AMPLITUDES IN TIME-DEPENDENT CALCULATIONS

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Solution of the time-dependent Schrödinger equation for ionization processes offers advantages over time-independent methods in that the asymptotic boundary conditions need not be imposed upon the solutions. Rather, wave functions are propagated forward in time and unitarity insures that exponentially growing components are not present. For charged particles there is the additional advantage that the logarithmic phase factors do not enter explicitly. For these reasons, computation of ionization by direct solution of the time-dependent Schrödinger equation is growing in popularity.

Despite these considerable advantages, it proves difficult to extract the ionization amplitude since there are three (or more) charged particles in the final state. Separation of ionization and excitation is also problematical owing to Rydberg series of bound states converging to the ionization threshold. In essence, a clean separation between ionization and excitation charge transfer does not emerge until large times.

Solov'ev[3] has identified a phase factor that is present in time-dependent wave functions, namely the factor

$$\exp[-ir^2/2t] \tag{1}$$

which oscillates rapidly as a function of the variable r. This rapid oscillation represents a significant complication for direct solutions at large times since it is necessary to use a small grid spacing to follow them accurately. Alternatively, it is possible to exploit this oscillatory factor to obtain a simple expression for the ionization amplitude. This has been done in our time-dependent calculations using the Sturmian method and scaled coordinates; however, the procedure for extracting ionization amplitudes is not limited to the Sturmian representation.

By projecting wave functions $\varphi(\tau, \mathbf{q})$ in scaled coordinates onto plane waves, we find that the ionization amplitude is given by

$$|A(\mathbf{k})| = |\varphi(0, \mathbf{k}/v)| \tag{2}$$

for single ionization by heavy particles moving with velocity v. This result can be written in conventional coordinates as

$$|A(\mathbf{k})| = \lim_{t\to\infty} |\psi(t, \mathbf{k}t)|. \tag{3}$$

These equations give a simple means of extracting ionization amplitude from coordinate-space wave functions. The procedure has been verified for a solvable model[4] where the ionization amplitude was computed earlier by the more conventional expression[5]

$$A(\mathbf{k}) =< \psi_{\mathbf{k}}^{(out)}(t)|\psi_i^{(in)}(t) > . \tag{4}$$

The solvable model also suggests that the limit expression for the magnitude of the amplitude is reached at values of time that are not prohibitively large.

Our simple expression for the ionzation amplitude can be generalized to fragmentation of a system into any number of particles. It is only necessary to replace the coordinates by their classical counterpart in a field-free region, namely, $\mathbf{r}_i = \mathbf{k_i} t/m_i$, and take the limit as t becomes infinite.

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