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SCHRODINGER EQUATION FOR SCATTERING WITH ENERGY LOSS

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Abstract:

An attempt is made to establish a model Schrödinger equation for the description of heavy ion scattering with energy loss. This equation is linear and can be related to the quantal coupled channels approach. A possible parametrization of the model Hamiltonian is considered.

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Schrödinger equation with an energy-losing potential. Energy non-conservation in the Schrödinger picture can be connected with an explicit time dependence of the scattering potential between two heavy ions:

\[ (-i \partial / \partial t - \nabla^2 / 2m + V + V^L(t)) \phi(r, t) = 0. \]  

(1)

To describe energy loss in the relative motion owing to internal excitation, the energy-losing potential \( V^L \) must contain only positive frequencies,

\[ V^L(t) = \int_{\omega}^{\infty} \tilde{V}^L(\omega) e^{i \omega t} d\omega. \]  

(2)

Transforming eq. (1) to the energy dependent form

\[ (E + \frac{\nabla^2}{2m} - V) \tilde{\phi}(r, E) = \int_{E'}^{\infty} \tilde{V}^L(E' - E) \tilde{\phi}(r, E') dE'. \]  

(3)

we see indeed that the term \( \tilde{V}^L(\omega), \omega > 0 \), appears in a source term via which current from wave function components \( \tilde{\phi}(r, E') \) with energy \( E' \) is fed into components \( \tilde{\phi}(r, E) \) with the lower energy \( E = E' - \omega \), thus describing energy loss.

The initial condition for the solution of eq. (1) is that it start out as a free normalized wave packet with mean momentum \( k_0 \). The corresponding boundary condition for eq. (3) is that the solution \( \tilde{\phi}(r, E) \) must consist of an incident free wave at energy \( E_0 \)

\[ \phi^\circ_{k_0}(r, E) = \left[ \Delta(E - E_0) \right] \frac{1}{k_0} e^{i k_0 r} \]  

(4)

plus terms at all energies which asymptotically purely outgoing. Here \( \Delta(x) \) is a narrow distribution about \( x = 0 \), normalized to unity. Equation (3)
automatically restricts the solution to energies \( E \leq E_0 \), as is most easily seen by a perturbation theory argument. Asymptotically we have

\[
\phi(r, E) \rightarrow \left[ \Delta(E - E_0) \right]^{1/2} e^{i \frac{\mathbf{k} \cdot \mathbf{r}}{\hbar}} + F(\Omega, E) \frac{e^{i k r}}{r} \tag{5}
\]

where the scattering amplitude \( F(\Omega, E) \) determines the differential cross section per unit energy for final energies \( E \leq E_0 \):

\[
\frac{d^2 \sigma}{d \Omega \, dE} = \frac{k}{k_0} \left| F(\Omega, E) \right|^2. \tag{6}
\]

The requirement that during scattering the wave may lose energy but not probability current, implies

\[
\int_{E_0}^{E} dE \left( \langle \tilde{\phi}(E) , \text{Im} \nabla \phi(E) \rangle + \text{Im} \langle \tilde{\phi}(E), \int dE' \nabla^L(\bar{E}', E) \tilde{\phi}(E') \rangle \right) = 0. \tag{7}
\]

The second term in eq. (7) receives contributions only from those components in the bra \( \langle \tilde{\phi}(E) \) which have energy \( E < E_0 \), and contain only outgoing waves; thus

\[
\int_{E_0}^{E} dE \left( \langle \tilde{\phi}(E) , \text{Im} \nabla \phi(E) \rangle \right) = - \int_{E_0}^{E_0} dE \left( \int dE'' \langle \tilde{\phi}(E'') , \nabla^L(\bar{E}'', E) \text{Im} G^+(E) \int_{E}^{E_0} dE' \nabla^L(\bar{E}', E) \phi(E') \rangle \right), \tag{8}
\]

where \( G^+(E) = (E + i \eta - T - V)^{-1} \). Since the r.h.s. of eq. (8) is negative, we see that the introduction of the energy losing potential \( \tilde{V}^L(\tau, \omega) \) requires the presence of absorption in the energy conserving potential, \( \text{Im} V < 0 \). This has a natural interpretation (cf. eq. (3)): the wave component \( \tilde{\phi}(E) \) at energy \( E \) receives current influx via the source term from components \( \tilde{\phi}(E') \) at higher channel energies \( E' > E \); but since in turn this wave component \( \tilde{\phi}(E) \) appears again in the source term for components \( \tilde{\phi}(\bar{E}) \) with \( \bar{E} < E \), feeding current into the latter, this current loss for \( \tilde{\phi}(E) \) must be accounted for by an absorptive part in the energy conserving potential \( V \).
Condition (7) reads in the time dependent description
\[ \int_{-\infty}^{\infty} dt \langle \phi(t), (\text{Im } V + \text{Im } V^L(t)) \phi(t) \rangle = 0, \]
which implies, using eq. (1), the conservation of probability:
\[ \langle \phi(t), \phi(t) \rangle_{t=\infty}^{t=-\infty} = 0. \]

The condition of probability conservation thus gives rise to a relation between the energy losing potential \( V^L \) and the absorptive part of the energy conserving "optical" potential. This relation is rather indirect, however, as it involves the wave functions and an integral over channel energies or equivalently, time. An analogous relation between the imaginary part of the optical potential and the friction force appears in the perturbation theory of nuclear friction.\(^2\)

The appearance of a complex potential in the Schrödinger equation (1) makes the latter time reversal non-invariant. This irreversibility arises from the circumstance that the energy loss is built into the equation itself (rather than into the boundary condition on the solution) by demanding that \( V^L \) contain only positive frequencies.

**Coupled channels approach.** It is interesting to note that eq. (3) is closely analogous to the usual system of coupled elastic and inelastic channels,
\[ (E_0 - \epsilon_\mu - T - V^L_{\mu}) \psi_\mu = \sum_{\nu \neq \mu} V^L_{\mu \nu} \psi_\nu, \]
where the \( \psi_\mu \) are the channel wave functions and \( \epsilon_\mu \) is the internal excitation energy of the fragments. Ordering the channel labels according to increasing excitation energy \( \epsilon_\mu \) (with degeneracies taken care of appropriately), we can eliminate, in the equation for a given channel \( \mu \), the coupling to all channels with lower channel energy \( E_\nu = E_0 - \epsilon_\nu \), \( E_\nu < E_\mu \).
i.e. higher excitation energy $\epsilon_\nu > \epsilon_\mu$ and obtain

$$
(E_\mu - \mathcal{T} - \mathcal{V}_\mu(E_\mu))\psi_\mu = \sum_{\nu < \mu} \mathcal{V}_{\mu\nu}(E_\mu) \psi_\nu,
$$

(11)

with

$$
\mathcal{V}_\mu(E) = \mathcal{V}_{\mu\mu} + \sum_{\nu > \mu} \mathcal{V}_{\mu\nu} \left( \frac{1}{E^+ - E + \epsilon_\mu - H} \right) \mathcal{V}_{\nu\nu},
$$

(12)

$$
\mathcal{V}_{\mu\nu}(E) = \mathcal{V}_{\nu\mu} + \sum_{\nu > \mu} \mathcal{V}_{\mu\nu} \left( \frac{1}{E^+ - E + \epsilon_\mu - H} \right) \mathcal{V}_{\nu\nu}.
$$

(13)

In eq. (11) the channels are coupled via a triangular coupling matrix. The elastic channel $\mu = 0$ is uncoupled, and is described by the optical-model equation

$$
(E_0 - \mathcal{T} - \mathcal{V}_0(E_0))\psi_0 = 0,
$$

(14)

where the optical potential $\mathcal{V}_0$ is given by eq. (12) with $\mu = 0$ (Feshbach's generalized optical potential \textsuperscript{3}), but would in practice be constructed phenomenologically. The first inelastic channel is explicitly coupled only to the elastic channel, but loses current to the second, third etc. channels via the imaginary part of $\mathcal{V}_{11}$. So it goes down to the last open channel with $E_\mu = 0$. The optical potential $\mathcal{V}_\mu(E)$ in channel $\mu$ (eq. (12)) at energy $E_\mu = E$ is quite similar in structure to the optical potential in the elastic channel, $\mathcal{V}_0(E)$. In the coupling terms $\mathcal{V}_{\mu\nu}$ we neglect the sum on the r.h.s. of eq. (13) since, in contrast to the analogous sum in eq. (12), it consists of terms with indefinite sign. Thus we write $\mathcal{V}_{\mu\nu}(E) \approx \mathcal{V}_{\mu\nu}$ in eq. (11).

In typical inelastic heavy ion scattering situations the number of channels to be included in the system (11) is very large. Going over to a
continuous distribution of channel energies we may write

\[(E_0 - \epsilon + T - U_0 (E_0 - \epsilon)) \phi_\epsilon = \int \bar{V}^L(\epsilon, \epsilon') \phi_{\epsilon'}, d\epsilon', \]  

(15)

where the "channel density wave function"

\[\phi_\epsilon = \sqrt{\overline{\sigma}(\epsilon)} \overline{\Psi}_\mu(r)\]  

(16)

is the average of the usual channel wave function in the interval \(\epsilon - d\epsilon < \epsilon < \epsilon + d\epsilon\) multiplied by the square root of the average number of channels per unit excitation energy. The integral kernel on the l.h.s. of eq. (15) is

\[\bar{V}^L(\epsilon, \epsilon') = \sqrt{\overline{\sigma}(\epsilon)} \bar{V}(r; \epsilon, \epsilon') \sqrt{\overline{\sigma}(\epsilon')}, \epsilon > \epsilon',\]  

(17)

where \(\bar{V}(r; \epsilon, \epsilon')\) is some average matrix element of the internuclear interaction taken between internal states with excitation energies \(\epsilon\) and \(\epsilon'\). If one simply sets \(\bar{V}^L(\epsilon, \epsilon') = \bar{V}^L(\epsilon - \epsilon')\), then with \(E_0 - \epsilon = E, E_0 - \epsilon' = E'\),

\[(E + T + U_0 (E)) \phi_\epsilon = \int_{E'}^{E} \bar{V}^L(E' - E) \phi_{\epsilon'}, dE'.\]  

(18)

Identifying \(\phi_\epsilon(r)\) with \(\tilde{F}(r, \epsilon)\), we find that eq. (18) is the same as eq. (3) (the integral in eq. (3) is effectively cut off at \(E' = E_0\), owing to condition (4)). The square of the outgoing part of the channel density wave function (16) yields the scattering cross section per unit excitation energy, as in eqs. (5) and (6). The energy conserving optical potential \(U_0(E) \approx U_\mu(E)\) is complex and time reversal non-invariant because in rearranging the original time reversal invariant system (10) to obtain eq. (11), the boundary condition of outgoing waves in all channels with lower channel energy has been incorporated in \(U_\mu(E)\). The current conservation relation (7) follows from the hermiticity of the original coupled channels problem (10). We see that in physical content, the "smoothed-out" coupled channels problem (18) is closely anal-
ogous to a linear (as opposed to ref. 5) Schrödinger equation with a time dependent potential.

Application to heavy ion scattering. In heavy ion scattering at higher energies, transfer reactions with exchange of only a few mass or charge units may still be regarded as "quasi-inelastic" events. Channels involving substantial rearrangements as well as nondirect and "fusion" processes may be accounted for by an additional absorptive term in the energy conserving potential \( V \) of eq. (1) or (3). Then, of course, the equality sign in eq. (9) must be replaced by a "greater than" sign.

For actual calculations, the potentials in eq. (3) have to be parametrized phenomenologically. The energy conserving potential \( V(r) = \mathcal{V}_0(r,E) \) might be chosen equal to some current optical potential describing elastic heavy ion scattering (plus the Coulomb potential). Giving it a dependence on channel energy may account for differences between entrance and exit channels. The energy losing potential \( \mathcal{V}_L(r,E' - E) \) may be surmised to have the spatial dependence of the imaginary part of the optical potential; if it is spherical, energy is lost while angular momentum is conserved. Its dependence on \( \omega = E' - E > 0 \) might be that of a decreasing exponential, \( \mathcal{V}_L(r,E' - E) \propto \mathcal{V}_L(r) \exp[-(E' - E)/\Delta] \); for given \( E \), the coupling is to channels with higher \( E' > E \) only, and as \( E' \) is increased away from \( E \) (i.e. the internal excitation energy \( E' \) is decreased away from \( E \)) there is ever less overlap in the coupling matrix elements of eq. (17); moreover, the channel density \( \mathcal{F}(\epsilon') \) decreases exponentially. One would expect \( \Delta \) to be less than a few MeV, so that the coupling is between channels with neighboring energies. Besides on the difference \( E' - E \), \( \mathcal{V}_L \) will presumably also depend on the channel energy \( E \) itself. We may take \( \mathcal{V}_L \) as real and assign a smoothly varying sign to it (perhaps negative, in extrapolation from \( \mathcal{V}_L(r,\omega \to 0) \), where it becomes the average nuclear interaction). Although \( \mathcal{V}_L \) arises from a large sum of almost random matrix elements, it should vary smoothly since it appears
in eq. (18) where the channel density wave functions on the left- and right-hand sides have, by our choice, smoothly varying phases (extending the considerations of ref. 4 on the phases of the channel functions to the whole range of excitation energies). As to the magnitude of $V^L(\gamma)$, a very crude estimate based on eq. (8) yields

$$\left(\frac{V^L}{\Delta}\right)^2 \leq \frac{300}{(A^{1/3} + A^{1/3})} \frac{1}{A_{red}^{3/2}} \frac{1}{\sqrt{E_0}} \left| \text{Im} \frac{V}{(M_eV)^2}\right|$$

where $V^L$ is the mean strength of $V^L(\gamma)$.

Numerically, one would reduce eq. (18) to a discrete system of coupled equations whose number depends on the step width one chooses for the energy integration. Since the coupling matrix is triangular, no matrix inversion is required, i.e. the separate "channels" are computed one after the other in order of decreasing channel energy, starting with the elastic channel at energy $E_0$. A "channel" at energy $E$ couples explicitly only to those with $E' > E$ while the coupling to channels with $E' < E$ (including the closed ones) is implicit, via the properties of the potential $U_0$ which are determined phenomenologically. One may do the calculation by partial wave decomposition, but it would certainly be helpful if current semi-classical methods could be extended to the case of complex, time dependent (or energy losing) potentials considered here. On the other hand, it is clearly not evident at this point whether our way of treating inelastic scattering, which simultaneously describes energy loss and absorption, will in some limit reduce to the classical picture of friction with a force proportional to the velocity.

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References


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