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TIME INDEPENDENT WAVE PACKET THEORY OF COLLISIONS

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1. Introduction

The results briefly described in this lecture are the product of a many year collaboration with M. A. Nagarajan, Y. Abe, P. Amiot, C. Noble and I. J. Thompson. Three main aspects can be listed, namely i) a wave packet representation of channels and reaction mechanisms, ii) a variational approach to the calculation of transition amplitudes and iii) a mean field approximation. The theory has now reached a stage where practical calculations of reasonable approximations to many-body collision amplitudes become available.

2. The wave packet representation

The physical system under study is an N-particle system with coordinates $\underset{\sim}{r}_i$, momenta $\underset{\sim}{p}_i$ and masses m_i, $i = 1 \ldots N$ respectively. The wave packets introduced in this theory are specifically designed to accomodate many-body calculations : they have to be products of single particle wave packets. In momentum representation, for instance, we consider :

$$\chi(\underset{\sim}{p}_1 \ldots \underset{\sim}{p}_N) = \mathcal{A}\, \chi_1(\underset{\sim}{p}_1) \ldots \chi_N(\underset{\sim}{p}_N), \qquad (2.1)$$

where the χ_i's can be Gaussians for instance. The operator $\mathcal{A}$ is a product of symmetrizors and/or antisymmetrizors when bosons and/or fermions are considered. It will be omitted for simplicity in the following.

The factorization of many-body integrals provided by the representation $\{\chi\}$ is an enormous advantage in practical calculations. It is also known that the set $\{\chi\}$ makes an (overcomplete) set in the Hilbert space. These two advantages may seem contradictory, however, with the fact that the physics under study is usually not related to single particle properties. Most often the physics focusses on one (or several) observables $R_\alpha(\underset{\sim}{r}_1 \ldots \underset{\sim}{r}_N, \underset{\sim}{p}_1 \ldots \underset{\sim}{p}_N)$ and/or their conjugate observables $P_\alpha(\underset{\sim}{r}_1 \ldots \underset{\sim}{r}_N, \underset{\sim}{p}_1 \ldots \underset{\sim}{p}_N)$ and the temptation is great to set up a formalism in terms of R_α, P_α and complementary variables ξ, π rather than the initial variables $\{\underset{\sim}{r}_i, \underset{\sim}{p}_i\}$.

There is in fact no need to face the unwieldy transformation $\{\underset{\sim}{r}_i, \underset{\sim}{p}_i\} \Longleftrightarrow \{R_\alpha, P_\alpha, \xi, \pi\}$ and the technical complications related to this change of representation. There are many cases where a displacement and boosting operation :

$$\chi \Longrightarrow \bar{\chi} = \exp[i(k_\alpha R_\alpha - s_\alpha P_\alpha)]\, \chi, \qquad (2.2)$$

just transforms χ into an other wave packet $\bar{\chi}$ whose structure is as simple as that of χ. The parameters k_α, s_α which label $\bar{\chi}$ actually provide all the necessary physical information to specify initial and final conditions of experiments. Intermediate states, of

course, can as well be described in terms of $\bar{\chi}$.

Last but not least, wave packets remain in the Hilbert space. The aim of a theory being to provide finite numbers, the use of flexible and bounded wave functions is likely to help improving the accuracy and convergence of numerical calculations. As will be seen in the next section, there is no major difference between collision (continuum) problems and bound state problems, for a wave packet remains square integrable while it goes to infinity or remains at a finite distance.

3. Variational approach

All the information demanded by a theory of an atomic or nuclear system may be recovered if the matrix elements of the Green's function are known. Let $\mathcal{H}$ be the hamiltonian of the N-body system. A collection of matrix elements :

$$\mathcal{D} = \langle \chi' | (E + i\Gamma - \mathcal{H})^{-1} | \chi \rangle, \qquad (3.1)$$

or in a slightly more complicated formalism, of matrix elements :

$$\mathcal{T} = \langle \chi' | V' (E + i\Gamma - \mathcal{H})^{-1} V | \chi \rangle, \qquad (3.2)$$

obviously provide the Fourier transform of the evolution operator, or even more explicitly the off-shell T-matrix. Here χ and χ' are any product-type wave packet such as shown in eq. (2.1). They could be of the type shown by eq. (2.2) as well. If R_α is a distance between

centers-of-mass, and P_α the corresponding momentum, $\bar{\chi}$ is furthermore an excellent approximation to a channel wave function (a boosted shell model).

In eqs. (3.1) and (3.2) an imaginary part $i\Gamma$ is added to the energy E in order to allow an on-shell limit $\Gamma \to 0$. When E is in a range of bound states, poles of $\mathcal{D}$ or $\mathcal{T}$ give information on bound states. When E is in the continuum, one deals with a theory of collisions, obviously (in eq. (3.2) V and V' are prior and post potentials). All told the inversion of $(E + i\Gamma - \mathcal{H})$ is the only technical problem to face.

As long as Γ is finite the Green's function acting on a wave packet χ (or $V\chi$) gives again a wave packet. Consider the functional :

$$F \equiv \langle \Phi' | \chi \rangle + \langle \chi' | \Phi \rangle - \langle \Phi' | (E + i\Gamma - \mathcal{H}) | \Phi \rangle, \qquad (3.3)$$

where Φ and Φ' are infinitely flexible wave packets. Variation and stationarity of F with respect to Φ and Φ' prove, trivially, that the stationary value of F is nothing but $\mathcal{D}$. An identical variational principle is obtained for $\mathcal{T}$ if V and V' are inserted in F.

The Green's function between wave packets can thus be calculated variationally with just wave-packet trial functions. The on-shell limit can be taken later.

In the next section we show how mean-field approximations, very convenient for practical calculations, can be implemented in this wave packet scheme.

4. Mean fields

Nothing prevents to restrict Φ, Φ' in eq. (3.3) to factorizable wave packets analogous to χ and $\bar{\chi}$. Then Φ and Φ' are no more infinitely flexible, but the resulting approximations $\bar{\mathcal{D}}$ to $\mathcal{D}$ (or $\bar{\mathcal{T}}$ to $\mathcal{T}$) are nonetheless of great interest.

This is because F contains a term (the last one) which is close to the Rayleigh-Ritz functional. Hence the ansatz :

$$\Phi = \mathcal{A} \prod_i \varphi_i, \tag{4.1a}$$

$$\Phi' = \mathcal{A} \prod_i \varphi_i', \tag{4.1b}$$

generates from F a simple generalization of Hartree Fock equations. A slightly detailed argument shows that one must solve equations of the form :

$$(\eta_i - h)\varphi_i = S_i, \tag{4.2a}$$

$$\varphi_i' (\eta_i - h) = S_i', \tag{4.2b}$$

where h is the usual Hartree Fock hamiltonian and S_i, S_i' are source terms derived for the first two terms of F. Preliminary results show that this approximation can be excellent. For more details the reader is referred to 1) and 2).

5. Conclusion

Time independent wave packets are of major interest for microscopic calculations of the Green's function, for all the many-body integrals can be made factorizable. Both the initial and final conditions are kept under control by the variational method we have introduced. This contrasts with time dependent methods, where usually numerical approximations are non linear and thus

incompatible with the linear superposition of channels.

It is a pleasure to thank the organizers of this Symposium for this opportunity of stimulating and encouraging exchanges.

REFERENCES

1) B. G. Giraud, M. A. Nagarajan and I. J. Thompson, Annals of Physics (N. Y.) 152 (1984) 475

2) Y. Abe and B. G. Giraud, Nuclear Physics A440 (1985) 311