# Elementary deconvolution method for the wave packet theory of collisions

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The $T$ matrix is more easily calculated when the initial and final channels are described in terms of a basis of wave packets for the relative motion. Usual channels, however, describe relative motion in terms of pure plane waves. We give a fast and practical connection between the latter and the former representations.

## I. INTRODUCTION

Consider a projectile "$a$" with degrees of freedom $\mathbf{r}_1,\ldots,\mathbf{r}_a$ for its single-particle constituents. The corresponding Jacobi coordinates are the internal degrees of freedom $\xi_1,\ldots,\xi_{a-1}$ and the projectile center-of-mass (c.m) coordinate $\mathbf{R}_a$. In the following, the conjugate momenta to these degrees of freedom will be denoted $\mathbf{p}_1,\ldots,\mathbf{p}_a$, $\pi_1,\ldots,\pi_{a-1}$, and $\mathbf{P}_a$, respectively.

With obvious notations we will also use the degrees of freedom $\mathbf{r}_{a+1},\ldots,\mathbf{r}_{a+A}$, $\xi_{a+1},\ldots,\xi_{a+A-1}$, $\mathbf{R}_A$, and $\mathbf{p}_{a+1},\ldots,\mathbf{p}_{a+A}$, $\pi_{a+1},\ldots,\pi_{a+A-1}$, $\mathbf{P}_A$ for the coordinates and momenta of a target "$A$," respectively. A standard recombination of $\mathbf{R}_a,\mathbf{R}_A,\mathbf{P}_a,\mathbf{P}_A$ defines the relative and total c.m. coordinates and momenta $\mathbf{r}$, $\mathbf{R}$, $\mathbf{p}$, and $\mathbf{P}$, respectively.

A channel is then described by the wave function

$$\Psi_{nq}(\xi,\mathbf{r},\mathbf{R})=\psi_{n_a}(\xi_1,\ldots,\xi_{a-1})\psi_{n_A}(\xi_{a+1},\ldots,\xi_{A+a-1})\times\Gamma(\mathbf{R})\exp(i\mathbf{q}\cdot\mathbf{r})\ , \tag{1.1}$$

or its analog in terms of Jacobi momenta. In Eq. (1.1) the labels $n\equiv(n_a,n_A)$ are spectroscopic labels, the wave functions $\psi$ are the corresponding projectile and target internal wave functions, the c.m. state $\Gamma$ can be anything as long as its factorization ensures Galilean invariance of the theory, and finally the label $\mathbf{q}$ appears in a pure plane wave for relative motion, normalized to unit flux.

The difficulties raised by the use of Jacobi coordinates in this representation, Eq. (1.1), when practical calculations are at stake (not to mention antisymmetrization), are obvious and well documented.[1] This is why we have introduced a microscopic[2] representation of channels,

$$\chi_{n\mathbf{ks}}(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{R}_a)\exp(-i\mathbf{s}_a\cdot\mathbf{P}_a)\varphi_{n_a}(\mathbf{r}_1,\ldots,\mathbf{r}_a)\exp(-i\mathbf{k}\cdot\mathbf{R}_A)\exp(-i\mathbf{s}_A\cdot\mathbf{P}_A)\varphi_{n_A}(\mathbf{r}_{a+1},\ldots,\mathbf{r}_{a+A})\ , \tag{1.2}$$

where static shell-model wave functions $\varphi_{n_a}$ and $\varphi_{n_A}$ are suitably boosted and shifted by means of the exponentials of the one-body operators $\mathbf{R}_a,\mathbf{P}_a$ and $\mathbf{R}_A,\mathbf{P}_A$. Hence single-particle orbitals are individually boosted and $\chi_{n\mathbf{ks}}$ retains all the factorization properties which make $\varphi_{n_a}$ and $\varphi_{n_A}$ handy wave functions. In particular, if $\varphi_{n_a}$ and $\varphi_{n_A}$ are Slater determinants, a straightforward antisymmetrization of the theory makes $\chi_{n\mathbf{ks}}$ a simple Slater determinant also.

We have thus shown in our previous paper[3] that the calculation of a matrix element of the operator

$$T=V+V'GV\ , \tag{1.3}$$

where $V'$ and $V$ are the post and prior potential operators, respectively, and $G\equiv(E-H)^{-1}$ is the full Green's function of the Hamiltonian $H$, is tractable, *provided* one uses the representation provided by Eq. (1.2),

$$\mathscr{D}_{\mathbf{k}'s'\mathbf{ks}}=\langle\chi_{\mathbf{k}'s'}\mid T\mid\chi_{\mathbf{ks}}\rangle\ . \tag{1.4}$$

(The spectroscopic labels $n$ are most often omitted in the following.) Clearly, the advantage of the representation, Eq. (1.4), with respect to the traditional representation

$$T_{\mathbf{q}'\mathbf{q}}=\langle\Psi_{\mathbf{q}'}\mid T\mid\Psi_{\mathbf{q}}\rangle\ , \tag{1.5}$$

is that single particle degrees of freedom may be used throughout Eqs. (1.2)—(1.4), while Jacobi coordinates plague Eqs. (1.1) and (1.5).

The connection between a wave function $\chi_{\mathbf{ks}}$ and a wave function $\Psi_{\mathbf{q}}$, however, is not trivial. Nonspurious shell-model wave functions $\varphi$ are products of an internal wave function $\psi$ and a c.m. wave packet $\gamma$. If it were necessary to use Jacobi coordinates in Eq. (1.2), we would obtain

$$\chi_{n\mathbf{ks}}=\psi_{n_a}(\xi_1,\ldots,\xi_{a-1})\psi_{n_A}(\xi_{a+1},\ldots,\xi_{a+A-1})\times\exp[i\mathbf{k}\cdot(\mathbf{R}_a-\mathbf{R}_A)]\gamma_a(\mathbf{R}_a-\mathbf{s}_a)\gamma_A(\mathbf{R}_A-\mathbf{s}_A)\ . \tag{1.6}$$

It is clear from Eq. (1.6) that the product $\gamma_a\gamma_A$ of c.m.

 

wave packets also describes a static, zero-point motion of the total c.m. about the point $\mathbf{S}=(M_a\mathbf{s}_a+M_A\mathbf{s}_A)/M$, where $M_a$, $M_A$, and $M$ are the projectile, target, and total masses, respectively. It is also clear that the relative motion is described by a wave packet localized about the point $\mathbf{s}=(\mathbf{s}_a-\mathbf{s}_A)$, with an average momentum $\mathbf{k}$. As to internal structures, they are the same in Eqs. (1.6) and (1.1), which justifies the consideration of $\chi_{\mathbf{ks}}$ as a channel state.

In this paper we consider the case where the product $\gamma_a\gamma_A$ can be recombined as a product $\gamma\Gamma$ of wave packets for the relative motion and the total c.m., namely

$$\exp[i\mathbf{k}\cdot(\mathbf{R}_a-\mathbf{R}_A)]\gamma_a(\mathbf{R}_a-\mathbf{s}_a)\gamma_A(\mathbf{R}_A-\mathbf{s}_A)$$
$$=\exp(i\mathbf{k}\cdot\mathbf{r})\gamma(\mathbf{r}-\mathbf{s})\Gamma(\mathbf{R}-\mathbf{S})\ . \quad (1.7)$$

This property is exact (and familiar) in Gaussian models and it is a reasonable approximation in non-Gaussian models anyhow. It is clearly possible to choose the shifts $\mathbf{s}_a$ and $\mathbf{s}_A$ in such a way that $\mathbf{S}=0$; hence insertion of Eq. (1.7) into Eq. (1.6) yields

$$\chi=\psi\psi\Gamma\exp(i\mathbf{k}\cdot\mathbf{r})\gamma\ . \quad (1.8)$$

A comparison of Eqs. (1.8) and (1.1) shows that $\chi$ is nothing but $\Psi$, except for a cutoff form factor $\gamma$ in the space of relative motion,

$$\chi_{n\mathbf{ks}}(\xi,\mathbf{r},\mathbf{R})=\Psi_{n\mathbf{k}}(\xi,\mathbf{r},\mathbf{R})\gamma(\mathbf{r}-\mathbf{s})\ . \quad (1.9)$$

This result, Eq. (1.9), describes the connection between traditional channel wave functions $\Psi$ and our wave packet representation $\chi$. *The subject of this paper is to reconstruct a channel plane wave $\Psi$ as a sum of channel wave packets $\chi$'s,* in order to reconstruct an amplitude $T_{\mathbf{q}'\mathbf{q}}$, Eq. (1.5), as a sum of the more available amplitudes $\mathscr{D}_{\mathbf{k}'\mathbf{s}',\mathbf{ks}}$, Eq. (1.4).

In the case of a short range $V$, there is no need to reconstruct completely $\Psi$ in terms of the $\chi$'s, for only the function $V\Psi$ appears in the formalism. The reconstruction must span only the range of $V$ in order to provide a correct calculation of $T_{\mathbf{q}'\mathbf{q}}$ as regards the prior potential. An identical remark holds for the bra side of the calculation, $\langle\Psi'\mid V'$, where $\Psi'$ is the final plane wave and $V'$ the post potential.

This paper is thus organized as follows. In Sec. II we reduce the reconstruction problem in the interaction region, which is a three-dimensional volume, to three independent, one-dimensional reconstructions. We also prove that the reconstruction method may be made independent of the momenta $\mathbf{q}',\mathbf{q},\mathbf{k}',\mathbf{k}$, a clearly advantageous result. In Sec. III we show an explicit example of reconstruction, and a qualitative generalization of this example. A numerical application is provided in Sec. IV. Finally, Sec. V contains a discussion and conclusion.

## II. PRELIMINARY RESULTS

### A. Projection ansatz

As seen from Eq. (1.8), the only degree of freedom which raises concern is the relative distance $\mathbf{r}=\mathbf{R}_a-\mathbf{R}_A$, or its conjugate $\mathbf{p}$. The product $\psi\psi\Gamma$ will thus be understood in the following and it will be convenient to shorten Eq. (1.8) to

$$\chi_{\mathbf{ks}}=\exp(i\mathbf{k}\cdot\mathbf{r})\gamma_{\mathbf{s}}(\mathbf{r})\ , \quad (2.1)$$

with

$$\gamma_{\mathbf{s}}(\mathbf{r})\equiv\gamma(\mathbf{r}-\mathbf{s})=\pi^{-3/4}\beta^{-3/2}\exp[-\tfrac{1}{2}(\mathbf{r}-\mathbf{s})^2/\beta^2]\ , \quad (2.2)$$

where $\beta$ is the width of the relative motion wave packet.

We could follow the method of Peierls and Yoccoz[4] or that of Peierls and Thouless[5] [which are made equivalent here by the boost exhibited by Eq. (2.1)] and define a pure plane wave via the integral

$$\exp(i\mathbf{k}\cdot\mathbf{r})=\pi^{-3/4}(2\beta)^{-3/2}\int d\mathbf{s}\,\chi_{\mathbf{ks}}\ , \quad (2.3)$$

but this would induce a double integral expansion of $T_{\mathbf{k}'\mathbf{k}}$ in terms of $\mathscr{D}_{\mathbf{k}'\mathbf{s}'\mathbf{ks}}$. Much more practical for numerical application is a discretization of Eq. (2.3),

$$\exp(i\mathbf{k}\cdot\mathbf{r})\simeq\tilde{\Psi}_{\mathbf{k}}\equiv\sum_{j=1}^{N}c_j\chi_{\mathbf{ks}_j}\ , \quad (2.4)$$

where the weights $c_j$ are real and the shifts $\mathbf{s}_j$ must be chosen in such a way that the form factor

$$U(\mathbf{r})\equiv\exp(-i\mathbf{k}\mathbf{r})\tilde{\Psi}_{\mathbf{k}}=\sum_{j=1}^{N}c_j\gamma_{\mathbf{s}_j}(\mathbf{r})\ , \quad (2.5)$$

be as close as possible to unity when $\mathbf{r}$ is inside the interaction region. Then $U$ may be small and decaying outside of this region.

In the following we thus concentrate on the discretization ansatz, Eq. (2.4), which is actually an attempt to project a plane wave with momentum $\mathbf{k}$ onto the subspace spanned by the wave packets $\chi_{\mathbf{ks}_j}$. Equivalently, the projection ansatz, Eq. (2.5), describes an attempt to project the flat unit function $U(\mathbf{r})$ onto the subspace spanned by the zero-momentum wave packets $\gamma_{\mathbf{s}_j}(\mathbf{r})$.

### B. Three-dimensional factorization

Assume that $j$ in Eqs. (2.4) and (2.5) is a triple index, $j\equiv(\lambda\mu\nu)$ and that, accordingly, $c_j$ factorizes as $c_\lambda c_\mu c_\nu$ and $\mathbf{s}_j$ runs its three components separately, $\mathbf{s}_j\equiv(x_\lambda,y_\mu,z_\nu)$. Then, the number of wave packets $N$ factorizes as $N=N_xN_yN_z$ and Eq. (2.5) factorizes as

$$U(\mathbf{r})=U_x(x)U_y(y)U_z(z)\ , \quad (2.6)$$

where $\mathbf{r}\equiv(xyz)$ and

$$U_x(x)=\pi^{-1/4}\beta^{-1/2}\sum_{\lambda=1}^{N_x}c_\lambda\exp[-\tfrac{1}{2}(x-x_\lambda)^2/\beta^2]\ , \quad (2.7)$$

with analogous formulae for $U_y$ and $U_z$.

In the same way, the approximated plane wave $\tilde{\Psi}_{\mathbf{k}}$ in Eq. (2.4) factorizes as

$$\tilde{\Psi}_{\mathbf{k}}(r)=\tilde{\Psi}_{k_x}(x)\tilde{\Psi}_{k_y}(y)\tilde{\Psi}_{k_z}(z)\ , \quad (2.8)$$

with

$$\tilde{\Psi}_{k_x}(x)=\exp(ik_xx)U_x(x)\ , \quad (2.9)$$

and obviously analogous formulae for the $y$ and $z$ degrees

of freedom.

The search for optimal shift parameters $\mathbf{s}_j$ and expansion coefficients $c_j$, see Eqs. (2.4) and (2.5), can thus be reduced to the search of optimal *and one-dimensional* coefficients and shifts $c_\lambda$ and $x_\lambda$, see Eq. (2.7).

### C. Reduction to zero momentum

We first notice from Eq. (2.3) that the plane wave momentum $\mathbf{q}$ and the wave-packet average momentum $\mathbf{k}$ need not be different, since an expansion with respect to the shift $\mathbf{s}$ already takes advantage of a complete basis. In order to optimize the approximation $\tilde{\Psi}_\mathbf{k}$ generated by Eq. (2.4), we will minimize the fluctuation $\Delta k^2$ defined by

$$\langle \tilde{\Psi}_\mathbf{k} | \tilde{\Psi}_\mathbf{k} \rangle \Delta k^2 = \langle \tilde{\Psi}_\mathbf{k} | p^2 | \tilde{\Psi}_\mathbf{k} \rangle - \langle \tilde{\Psi}_\mathbf{k} | p | \tilde{\Psi}_\mathbf{k} \rangle^2 \tag{2.10}$$

with respect to the choice of the $c_j$'s and $\mathbf{s}_j$'s. (This fluctuation is a sum of three independent fluctuations, $\Delta k_x^2, \Delta k_y^2, \Delta k_z^2$, obviously.)

Since by definition, Eq. (2.5), $\tilde{\Psi}_\mathbf{k} = \exp(i\mathbf{k}\cdot\mathbf{r})U$, we find from elementary commutation rules and the finite range of $U$ that

$$\Delta k^2 = \langle U | p^2 | U \rangle \langle U | U \rangle^{-1} . \tag{2.11}$$

Hence the value of $\Delta k^2$ does not depend on $\mathbf{k}$ in this approximation. In the following we will concentrate on the optimization of $U$ as an approximation to the zero momentum wave.

## III. EXPLICIT CASES OF RECONSTRUCTION

In this section only one-dimensional models will be considered, as allowed by Sec. II B. The subscript $x$ will be omitted for simplicity.

### A. The two-wave-packet case

It is physically obvious that $U(x)$, a sum of two Gaussian in this special case, must be as flat as possible in order to minize $\Delta k^2$. Hence the two Gaussians will be added to each other with equal (positive) weights and the separation of their centers should be of the same order as their widths $\beta$. In momentum representation we set

$$U(p) = 2^{-1/2}\pi^{-1/4}\beta^{1/2}\exp(-\tfrac{1}{2}\beta^2\sigma^2) \times \{\exp[-\tfrac{1}{2}\beta^2(p-i\sigma)^2] + \exp[-\tfrac{1}{2}\beta^2(p+i\sigma)^2]\} . \tag{3.1}$$

It is seen that the center of each wave packet lies at $\pm\beta^2\sigma$ from the center of the interaction region in the coordinate space, and that

$$\langle U | U \rangle = 1 + \exp(-\beta^2\sigma^2) , \tag{3.2a}$$

$$\langle U | p^2 | U \rangle = \frac{1}{2\beta^2}\langle U | U \rangle - \sigma^2 \exp(-\beta^2\sigma^2) . \tag{3.2b}$$

The minimum of $\Delta k^2$ is reached for $\beta^2\sigma^2 = 1.28$ or $\beta\sigma = 1.13$, which corresponds to a separation distance, between wave packet maxima, equal to $2\beta^2\sigma = 2.26\beta$. The corresponding shape of $U$ is shown in Fig. 1. It is clearly far from a perfectly flat form factor, but definitely provides a much more uniform and broader coverage of an interaction domain than would a lone Gaussian centered at the origin. The bare value $1/2\beta^2$ of $\Delta k^2$ is reduced by 56%, a non-negligible result.

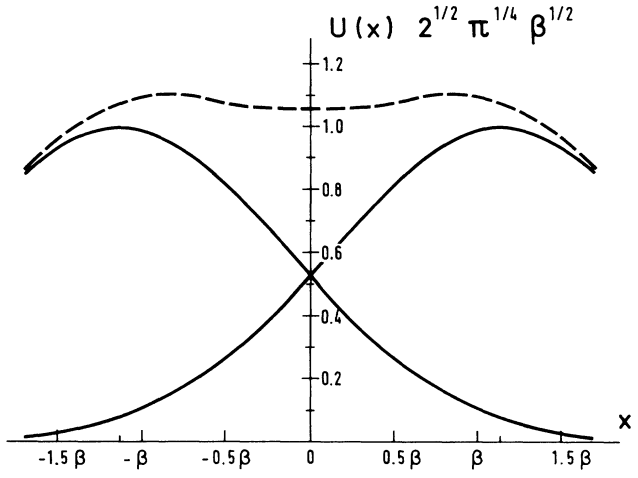


FIG. 1. Optimal reconstruction of a flat form factor $U$ by a recombination of two Gaussians.

Such an improvement with just two wave packets is of some value, for it leads to a similar improvement with just $2^3 = 8$, wave packets in the three-dimensional case. With also eight wave packets for the final channel, the $T$-matrix amplitude $T_{\mathbf{k}'\mathbf{k}}$ will thus be approximated by a coherent sum, with equal weights, of 64 wave packet amplitudes $\mathscr{D}_{\mathbf{k}'\mathbf{s}'\mathbf{k}\mathbf{s}}$. It will be noticed that, in units given by $2^{-1/2}\pi^{-1/4}\beta^{-1/2}$, the center value is $U_x(x=0) = 1.06$ when $\beta\sigma = 1.13$. In order to renormalize it to $U_x(x=0) = 1$, the correct physical value, it will thus be necessary to introduce a renormalization factor equal to the reciprocal, 0.94. With both an initial and a final channel, and three-dimensional calculations, the renormalization factor will then be $(1.06)^{-6}$.

### B. The three-wave-packet case

We now locate one wave packet at the center and the other two at a distance $\pm\beta^2\sigma$ from the center. The ansatz for $U$ is (with a prejudice for equal weights for the three packets)

$$U(p) = 3^{-1/2}\pi^{-1/4}\beta^{1/2}\exp(-\tfrac{1}{2}\beta^2p^2) \times [1 + \exp(i\beta^2\sigma p) + \exp(-i\beta^2\sigma p)] . \tag{3.3}$$

One finds, accordingly,

$$\langle U | U \rangle = 1 + \tfrac{4}{3}\exp(-\tfrac{1}{4}\beta^2\sigma^2) + \tfrac{2}{3}\exp(-\beta^2\sigma^2) , \tag{3.4a}$$

$$\langle U | p^2 | U \rangle = \frac{1}{2\beta^2}\langle U | U \rangle - \tfrac{1}{3}\sigma^2\exp(-\tfrac{1}{4}\beta^2\sigma^2) - \tfrac{2}{3}\sigma^2\exp(-\beta^2\sigma^2) . \tag{3.4b}$$

The minimum of $\Delta k^2$ is reached for $\beta^2\sigma^2=4.7$ or $\beta\sigma=2.17$, the distance between the centers of neighboring wave packets being now equal to $2.17\beta$, slightly smaller than the value $2.26\beta$ obtained for the two-wave-packet case. The bare value $1/2\beta^2$ of $\Delta k^2$ is now reduced by 70%, and it is clear that adding more, and suitably placed, wave packets to the expansion basis would decrease $\Delta k^2$ even further.

The value of $U$ at $x=0$ is now equal to 1.19, again in units specified by $3^{-1/2}\pi^{-1/4}\beta^{-1/2}$; hence a renormalization coefficient of $(1.19)^{-6}$ should be considered. Independent coefficients for the mixture of the three-wave-packet case should slightly diminish this value 1.19, a more flexible $U$ becoming flatter.

### C. Generalization

Consider an odd number of wave packets, $N_x'=2N_x+1$, with the $(N_x+1)$st packet centered at the origin and all packets equally spaced at distance $\beta^2\sigma$ from each other. We expect from the two previous subsections that this distance $\beta^2\sigma$ is of order $2.2\beta$. Indeed, at mid-distance, each Gaussian in a pair of nearest neighbors is then reduced to about 55% of its maximum, and hence the superposition of these nearest neighbors in that point reconstructs about 110% of the maximum of just one Gaussian. In other words, the Gaussians intersect roughly at midheight, which is a reasonable prescription to generate a flat $U$ on the average. The ansatz

$$U(x)=\sum_{j=-N_x}^{N_x}\exp-\frac{(x-j\beta^2\sigma)^2}{2\beta^2},\quad \beta\sigma\simeq 2.2 \tag{3.5}$$

thus generates a reasonably flat form factor $U$ in a range

$$\Delta x\simeq(2N_x+1)\beta^2\sigma\simeq(4.4N_x+2.2)\beta\ .$$

Accordingly, $\Delta p$ decreases as $\Delta x^{-1}$. The number of wave packets can be adjusted so that $\Delta x$ becomes larger than the diameter of the interaction region, or $\Delta p$ becomes smaller than the momentum resolution demanded by the problem under study. A slight improvement in the quality of $U$ may also be obtained by reinstating nonequal mixture coefficients $c_j$ in Eq. (3.5) and letting the Gaussians deviate slightly from equal spacing. These subtleties are disregarded in the following.

## IV. AN ILLUSTRATIVE EXAMPLE

Consider a Hamiltonian defined by its matrix elements

$$\langle p'\,|\,H\,|\,p\rangle=p^2\delta(p-p')-V_0\exp[-\nu^2(p^2+p'^2)]\ . \tag{4.1}$$

The separable nature of the potential, $V=-V_0\,|\,\nu\rangle\langle\nu\,|$, in obvious notation, makes it easy to calculate the $T$ matrix,

$$\begin{aligned}\mathscr{D}_{k'k}&\equiv\langle k'\,|\,T\,|\,k\rangle\\&\equiv\langle k'\,|\,(V+VGV)\,|\,k\rangle\\&=-V_0\langle k'\,|\,\nu\rangle\langle\nu\,|\,k\rangle(1-V_0\langle\nu\,|\,G\,|\,\nu\rangle)\ .\end{aligned} \tag{4.2}$$

In the wave packet representation, we get, in an analogous way,

$$\begin{aligned}\mathscr{D}_{\mathbf{k}'s'\mathbf{k}s}&\equiv\langle\chi_{\mathbf{k}'s'}\,|\,(V+VGV)\,|\,\chi_{\mathbf{k}s}\rangle\\&=-V_0\langle\chi_{\mathbf{k}'s'}\,|\,\nu\rangle\langle\nu\,|\,\chi_{\mathbf{k}s}\rangle(1-V_0\langle\nu\,|\,G\,|\,\nu\rangle)\ .\end{aligned} \tag{4.3}$$

Whatever the strength $V_0$ of the interaction, the dynamical factors $V_0(1-V_0\langle\nu\,|\,G\,|\,\nu\rangle)$ are the same in Eqs. (4.3) and (4.2). The quality of the reconstruction of $T_{k'k}$ in terms of $\mathscr{D}_{k's'ks}$ is thus entirely controlled by the quality of the reconstruction of $\langle\nu\,|\,\mathbf{k}\rangle$,

$$\langle\nu\,|\,\mathbf{k}\rangle\approx\sum_j c_j\langle\nu\,|\,\chi_{\mathbf{k}s_j}\rangle=\langle\nu\,|\,\exp(i\mathbf{k}\cdot\mathbf{r})\,|\,U\rangle\ . \tag{4.4}$$

In so far as $|\,\nu\rangle$, the form factor of the separable potential, has a range $\nu$ smaller or equal to the range $\frac{1}{2}\Delta x\simeq 2.2N\beta$ of the form factor $U$, this overlap, Eq. (4.4), is assumed to provide an excellent approximation.

For the sake of definiteness, consider the cases where $\beta=1.5$ fm, a typical value for a nuclear shell-model harmonic oscillator, and $\nu=1$ fm, a typical range for the nuclear force.

The formula

$$\begin{aligned}&\int dx\,\nu^{-1}\exp\left[-\frac{x^2}{4\nu^2}\right]\exp(ikx)\exp\left[-\frac{(x-s)^2}{2\beta^2}\right]\\&\quad=\pi^{1/2}\frac{2\beta}{(\beta^2+2\nu^2)^{1/2}}\exp\left[-\frac{s^2-4i\nu^2ks+2\beta^2\nu^2k^2}{2(\beta^2+2\nu^2)}\right]\end{aligned} \tag{4.5}$$

gives, as a special case,

$$\int dx\,\nu^{-1}\exp\left[-\frac{x^2}{4\nu^2}\right]\exp(ikx)=2\pi^{1/2}\exp(-\nu^2k^2)\ , \tag{4.6}$$

which corresponds to $\langle\nu\,|\,\mathbf{k}\rangle$. The quality of the approximation is thus good if

$$\rho\sum_j\frac{\beta}{(\beta^2+2\nu^2)^{1/2}}\exp\left[-\frac{(s_j-2ik\nu^2)^2}{2(\beta^2+2\nu^2)}\right]\approx 1\ , \tag{4.7}$$

where $\rho$ is that renormalization factor discussed at the end of Secs. III A and III B. (For instance, $\rho=0.94$ for two one-dimensional wave packets.)

For the one-dimensional case and two wave packets, the left-hand side of Eq. (4.7) takes on the values 0.98, 1.10, and 1.03 for $k=0$, 1, and 1.5 fm$^{-1}$, respectively, which is quite satisfactory. Then the approximation breaks down when $k\gtrsim 1.8$ fm$^{-1}$, because the oscillatory terms on that left-hand side are contradictory with the positive definite form factor $|\,\nu\rangle$ in the momentum representation; see Eq. (4.6). This spurious oscillation is clearly due to the finite range nature of the form factor $U(x)$ in coordinate space; hence our approximation is better at low momenta.

A similar result is found for three wave packets and the one-dimensional case. The left-hand side of Eq. (4.7) now takes the more weakly varying values 0.96, 1.00, and 1.31 for $k=0$, 1, and 1.8 fm$^{-1}$, respectively. This extends the

validity range of the approximation, as expected, even though an improvement of the normalization is clearly in order and can be implemented with more components in the reconstruction of $U$.

## V. DISCUSSION AND CONCLUSION

An expansion of a wave function in a basis of coherent wave packets is a familiar idea, which has already been considered in time dependent theories.[6] The semiclassical aspects, and advantages, of the wave packet representation, have already been stressed.[6,7] We have here used the same idea in a time independent theory.

The significant advantage of wave packets as basis states in a theory of collisions is the possibility of a shell-model representation of the initial and final channels and, hence, of a representation where microscopic (single particle) degrees of freedom are natural. This representation is then free of all complications concerning Jacobi coordinates and the unwieldy, related problem of antisymmetrization.

Channel wave functions, however, are plane waves (or distorted waves) with respect to the relative distance degree of freedom. We have shown in this paper how a plane wave, or that part of it which is pertinent to the interaction region, can be reconstructed as a coherent sum of wave packets. The optimal position of the wave packets and their respective admixture weights may be adjusted to the physical nature of the problem. We have selected, among other possible optimization rules, the minimization of the fluctuation $\Delta k^2$ of the relative linear momentum.

Our theory of collisions thus provides the collision amplitude as a coherent sum of amplitudes between wave packets. This allows the introduction of all the well-known, and powerful, shell model techniques into the theory of collisions.

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