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Approximation of velocity-dependent potentials
by separable kernels

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A B S T R A C T

The Schrödinger equation for a two-nucleon problem with velocity-dependent forces contains an integral operator; the kernel of this might be approximated by a separable kernel, then the equation can be easily solved. A method to construct the best separable approximation is given; the goodness of which is expressed in a simple way with the eigenvalues. It turns out that a reasonable approximation is possible if the first eigenvalue of the kernel is non-degenerate and widely separated from the next one. The properties of the approximation remain unchanged in momentum space representation.

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Introduction:

Assuming velocity-dependence ("non-locality") of the nucleon-nucleon force, the Schrödinger equation for the two-nucleon problem is this :

$$\Delta\psi + \nabla^2 - U(r)\psi + \Omega\psi = 0 \quad (1)$$

Here purely central forces are assumed. Ω is an operator which arises through quantization from a classical potential energy term

$$V(\vec{r}, \vec{p}) \longrightarrow V(\vec{r}, grad)$$

The exact velocity-dependence, and therefore the exact form of Ω is not known; but Ω is obviously linear and also hermit¹⁾.

While Ω is unknown, it is possible to write it in a standard form, i.e. as an integral transformation²⁾ with an hermit kernel.

1) Okubo and Marshak, Ann. of Phys. 4, 166-179 (1958).

2) This fact is tacitly used and can be proven rigorously.

See F. Riesz and B.Sz.-Nagy: Functional Analysis, Chapter V., no.90.

(1) then takes the form :

$$\Delta\psi + [k^2 - U(r)]\psi + \int_0^\infty K(r,r')\psi(r')dr' = 0 \quad (2)$$

with

$$K(r,r') = K^*(r',r)$$

$U(r)$ represents an ordinary velocity-independent ("local") force.

It is possible to include this term into the integral :

$$K'(r,r') = K(r,r') + \delta(r-r') U(r)$$

but such a step is purely formal and moreover destroys the continuity of the kernel, a property we want to use.

The equation (2) can be treated more easily if the kernel is "separable" 3) :

$$K(r,r') = h(r) h^*(r') \quad (3)$$

The following questions (largely of academical interest only) arise:

First: how can one find, for a given $K(r,r')$, the best separable approximation

$$K(r,r') \approx h(r) h^*(r') \quad ?$$

Second: how can one give a simple criterion for this best approximation to be also "good", so that it can be used as an approximation to the kernel in (2)?

Third: what happens to this approximation if we go over to momentum space representation - the procedure usually applied? ³⁾

The aim of the present paper is to answer these three questions.

³⁾ Yamaguchi, Phys. Rev. 95, 1628; Yamaguchi and Yamaguchi, Phys. Rev. 95, 1635.

1). Let be

$$\int_0^{\infty} \int_0^{\infty} K(r, r') K^*(r, r') dr dr' = K^2 < \infty \quad (4)$$

we want to find a function $h(r)$ such that

$$\int_0^{\infty} \int_0^{\infty} |K(r, r') - h(r) h(r')|^2 dr dr'$$

becomes a minimum, thus we define the "best" approximation in the sense of square deviation. It is well known from the theory of integral equations that $K(r, r')$ can be formally expanded into the - not necessarily convergent - series

$$K(r, r') = \sum_{n=1}^{\infty} \lambda_n U_n(r) U_n^*(r') ; \quad \int_0^{\infty} |U(r)|^2 dr = 1 \quad (5)$$

here $U_n(r)$ and λ_n are determined by the eigenvalue equation

$$\int_0^{\infty} K(r, r') U^*(r') dr' = \lambda U(r) \quad (6)$$

The expansion (5) will converge in the sense of square deviation;

if moreover the eigenvalues are all positive, or all negative,
 (5) will also converge in the strict sense. (Definite kernel.)
 The sequence $\{|\lambda_n|\}$ is bounded

$$|\lambda_1| \geq |\lambda_2| \geq \dots |\lambda_n| \geq \dots \quad (7)$$

and if there is an infinity of different eigenvalues (non-degenerate kernel), then

$$\lambda_n \longrightarrow 0 \quad (8)$$

To find the best separable approximation, we start from the relation valid for every $h(r)$

$$\left(\int_0^\infty h(r) h^*(r) dr - \lambda_1 \right)^2 \geq 0 \quad \text{i.e.}$$

$$\left[\int_0^\infty (h(r) h^*(r)) dr \right]^2 - 2\lambda_1 \int_0^\infty h(r) h^*(r) dr \geq -\lambda_1^2 \quad (9)$$

the first term on the r.h.s. can be written as

$$\int_0^\infty \int_0^\infty h(r) h^*(r) h(r') h^*(r') dr dr' \quad ;$$

the second term can be replaced, without upsetting the inequality, by the algebraically larger term

$$- 2 \int_0^{\infty} \int_0^{\infty} K(r, r') h(r) h^*(r') dr dr' ;$$

This follows from the Ritz variation principle which states

$$\left| \int_0^{\infty} h(r) \int_0^{\infty} K(r, r') h^*(r') dr' dr \right| \leq \left| \lambda_1 \int_0^{\infty} h(r) h^*(r) dr \right| \quad (10)$$

Carrying out these alterations, (9) can be written as

$$\int_0^{\infty} \int_0^{\infty} h(r) h^*(r) h(r') h^*(r') dr dr' - 2 \int_0^{\infty} \int_0^{\infty} h(r) h^*(r') K(r, r') dr dr' \geq -\lambda_1^2 \quad (11)$$

From (6) it can be easily verified that

$$-\lambda_1^2 = -2\lambda_1 \int_0^{\infty} \int_0^{\infty} K(r, r') U_1(r) U_1^*(r') dr dr' + \lambda_1^2 \int_0^{\infty} \int_0^{\infty} U_1(r) U_1^*(r) U_1(r') U_1^*(r') dr dr' \quad (12)$$

Finally we substitute $-\lambda_1^2$ from (12) into (11) and add

$$K^2 = \int_0^\infty \int_0^\infty K(r, r') K^*(r, r') dr dr'$$

to both sides; thus we obtain

$$\int_0^\infty \int_0^\infty |K(r, r') - \lambda_1 U_1(r) U_1^*(r')| dr dr' \geq \int_0^\infty \int_0^\infty |K(r, r') - \lambda_1 U_1(r) U_1^*(r')| dr dr' \quad (13)$$

Thus we have found the following result :

The best separable approximation is given by

$$h(r) h^*(r') = \lambda_1 U_1(r) U_1^*(r') \quad (14)$$

here λ_1 is the eigenvalue with maximum modulus of $K(r, r')$ and $U_1(r)$ one of the corresponding eigenfunctions. 4)

4) This result can be regarded as a special case of a general theorem of E. Schmidt. See Math. Ann. 65, pp. 370-399 (1908).

2). The question now arises - how good this best approximation is. As a measure for this we introduce the ratio
 [see (4)]

$$R_K = \frac{1}{K^2} \int_0^\infty \int_0^\infty \left| K(r, r') - \lambda_1 U_1(r) U_1^*(r') \right|^2 dr dr' \quad (15)$$

The calculation yields, as an immediate consequence of (5)

$$R_K = \frac{\sum_{n=2}^{\infty} \lambda_n^2}{\sum_{n=1}^{\infty} \lambda_n^2} = 1 - \frac{\lambda_1^2}{\sum_{n=1}^{\infty} \lambda_n^2} \quad (16)$$

Obviously R_K will be very small if $|\lambda_1|$ is very much larger⁵⁾ than the other eigenvalues.

From (16)

$$0 \leq R_K < 1 \quad (17)$$

5) It must be noted that we call "largest" the eigenvalue with maximum modulus; in a physical situation the eigenvalues are bound states with negative energy and thus our largest eigenvalue will correspond to the ground level.

follows. Thus we have two extreme cases: $R_K = 0$ implies $\lambda_2 = \lambda_3 = \dots = 0$, i.e. if we have only one eigenvalue, the approximation becomes exact and (5) yields

$$K(r, r') = \lambda_1 U_1(r) U_1^*(r')$$

(strictly separable kernel). It is important to notice that in the sequence

$$|\lambda_1| \geq |\lambda_2| \geq |\lambda_3| \geq \dots$$

each eigenvalue figures as often as its multiplicity indicates. Thus (18) implies also that λ_1 is a non-degenerate eigenvalue.

The other extreme case $R_K \approx 1$, occurs if the largest eigenvalues are closely spaced and particularly if the first eigenvalue has a degeneracy of high order.

To summarize: An hermitean kernel can be approximately factorized if its largest eigenvalue is non-degenerate and widely separated from the others; while a high order degeneracy of the largest eigenvalue makes such an approximate factorization impossible.

A simple example is the approximate factorization of the real symmetric kernel

$$K(r, r') = \begin{cases} r+r' & \text{if } 0 \leq r \leq 1, \quad 0 \leq r' \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

We have here

$$\lambda_1 = \frac{1}{2} + \frac{1}{\sqrt{3}} \quad U_1(r) = \frac{1 + \sqrt{3} r}{\sqrt{2} + \sqrt{3}}$$

$$\lambda_2 = \frac{1}{2} - \frac{1}{\sqrt{3}} \quad U_2(r) = \frac{1 - \sqrt{3} r}{\sqrt{2} - \sqrt{3}}$$

There are no other eigenvalues. The best approximation is

$$K(r, r') \approx \frac{\left(\frac{1}{2} + \frac{1}{\sqrt{3}}\right) (1 + \sqrt{3} r) (1 + \sqrt{3} r')}{2 + \sqrt{3}}$$

with

$$R_K = \frac{\left(\frac{1}{2} - \frac{1}{\sqrt{3}}\right)^2}{\left(\frac{1}{2} + \frac{1}{\sqrt{3}}\right)^2 + \left(\frac{1}{2} - \frac{1}{\sqrt{3}}\right)^2} \approx 0,006$$

a good approximation.

3). If the assumed nucleon-nucleon force is purely non-local ⁶⁾,
i.e. in (2)

$$U(r) \equiv 0$$

it is of advantage to treat the problem in momentum space representation. Then the integro-differential equation (2) becomes the pure integral equation

$$(p^2 + k^2) \tilde{\psi} + \int_0^\infty \tilde{K}(p, p') \tilde{\psi}(p') dp' = 0 \quad (19)$$

If, moreover, $\tilde{K}(p, p')$ is approximated by a separable kernel, (19) can be solved at once ³⁾.

The connection between coordinate and momentum space is given by

$$\begin{aligned} \tilde{\psi}(p) &= \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{pri} \psi(r) dr \\ \psi(r) &= \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{-pri} \tilde{\psi}(p) dp \end{aligned} \quad (20)$$

⁶⁾ As pointed out in the introduction, this is formally always the case, but then we are forced to include a delta function into the kernel, destroying its most useful properties.

We are going to show that the best separable approximation remains the best if we go over to momentum space and vice versa. Moreover the value of R_K remains unchanged.

Transforming (2) into momentum space (taking into account $U(r) \equiv 0$), we have

$$(p^2 + k^2) \tilde{\psi}(p) + \frac{1}{2\pi} \int_0^\infty \int_0^\infty K(r, r') e^{pri} \psi(r') dr' dr \quad (21)$$

or, expressing $\psi(r')$ from (20)

$$(p^2 + k^2) \tilde{\psi}(p) + \frac{1}{2\pi} \int_0^\infty \int_0^\infty \int_0^\infty K(r, r') e^{pri - p'r'i} \tilde{\psi}(p') dp' dr' dr \quad (22)$$

Comparing with (19) we find

$$\tilde{K}(p, p') = \int_0^\infty \int_0^\infty K(r, r') e^{(pr - p'r')i} dr dr' \quad (23)$$

(23) shows the following facts: Since $K(r, r')$ is hermitean, so is $\tilde{K}(p, p')$. If K is separable, $\tilde{K}$ is also separable. In particular, if

$$K(r, r') = h(r) h^*(r')$$

then

$$\widetilde{K}(p, p') = h(p) h^*(p')$$

with

$$\widetilde{h}(p) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} h(r) e^{pri} dr \quad (24)$$

We have to show that if $h(r)$ is a best separable approximation, the best similar approximation in momentum space is given by (24). Substituting (5) into (23), we have

$$\widetilde{K}(p, p') = \sum_{n=1}^{\infty} \frac{\lambda_n}{2\pi} \int_0^{\infty} U_n(r) e^{pri} dr \int_0^{\infty} U_n^*(r) e^{-p'r'i} dr' = \sum_{n=1}^{\infty} \lambda_n \widetilde{U}_n(p) \widetilde{U}_n^*(p') \quad (25)$$

From this, the eigenvalue equation

$$\int_0^{\infty} K(p, p') \widetilde{U}_n^*(p') dp' = \lambda_n \widetilde{U}_n(p) \quad (26)$$

follows. $U_1(r)$ is the first eigenfunction of K and therefore $\lambda_1 U_1(r) U_1^*(r')$ the best separable approximation to K , (26) indicates that $\widetilde{U}_1(p)$ is the first eigenfunction of $\widetilde{K}$ and thus $\lambda_1 \widetilde{U}_1(p) \widetilde{U}_1^*(p')$

the best separable approximation to $\tilde{K}$.

Finally (26) shows that the eigenvalues are not changed by transforming into momentum space. We can now define $R_K^{\sim}$ in exact analogy to R_K / see (15) and since both depend only on the -unchanged- eigenvalues, we have

$$R_K = R_K^{\sim}$$

With other words: the goodness of approximation is the same both in coordinate and in momentum space. The proof for a transformation from momentum space to coordinate space proceeds on exactly the same lines.

We conclude with the remark that all the statements are still true, if the kernel (and therefore the wave function) depends on $\vec{r}$ (and not on $|\vec{r}| = r$ only). The proofs remain exactly the same, but the integrations have to be understood over three variables. As pointed out earlier, the question of finding the best separable approximation to a given kernel is largely academical; besides the best approximation to the kernel does not necessarily guarantee the best approximation to the wave function. It is therefore interesting to point to a well-known result of Chew ⁷⁾ who derives from

⁷⁾ Chew, Phys. Rev. 93, 341 (1954).

a Schwinger's variational principle, results for the S-matrix corresponding to those described in this paper.

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