Holden-Day

Advanced

Physics

Monographs

Topics in Several Particle Dynamics

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HOLDEN-DAY, San Francisco, Cambridge, London, Amsterdam

Library of Congress Catalog Card Number: 67–13836
Printed in the United States of America

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Preface

There has recently been a surge of interest in theoretical questions concerning the quantum dynamics of a small number of particles, with the main emphasis on three-body problems. One reason for this may be the fact that computers are rapidly being developed to the point where we may begin to hope that reasonably accurate numerical solutions of Schrödinger's equation for three particles are attainable. In addition, spurred on by the work of Faddeev, we are beginning to understand how to overcome some of the tricky mathematical difficulties that are involved. There are many experimental situations, ranging from electron–hydrogen atom scattering to three-body resonances in high-energy physics, where a correct treatment of three- (and more) particle systems is essential to their understanding.

In this monograph, we have reviewed several techniques for treating three-particle systems (and other few-body systems) that have proved useful. We begin by surveying some mathematical aspects of the type of integral equations that arise in scattering theory. More details on Fredholm theory are left to the Appendix. Chapter 2 is concerned with some aspects of the two-body problem which are useful for the later discussion, while Chapter 3 treats the more general case of multi-channel two-particle systems. The question of rearranging the integral equations for scattering to make them more amenable to standard methods is studied in Chapter 4, and Chapter 5 deals with the three-body problem for factorable two-body potentials, where significant simplifications ensue. The integral equations to be solved have fewer variables if use is made of conservation of angular momentum, and the details of this analysis are given in Chapter 6, contributed by J. S. R. Chisholm. Finally, in Chapter 7, we describe several applications of variational principles, quite successful in practice, to problems of the type we have been discussing.

We hope that this monograph will help the reader with some knowledge of basic scattering theory to make the jump to the current literature on the subject. We regret that some topics have been omitted (in particular there is no discussion of relativistic problems), but in exculpation we cite the limitations of space and time.

The monograph has grown out of a series of lectures delivered by one of us (K. M. W.) in December, 1965, at Texas A and M University, and we thank Professor J. L. Gammel, the University, and the Air Force Office of Scientific Research for making these possible. We would also like to thank a number of scientists working in the field for helpful discussions, in particular, Professor J. L. Gammel, Professor A. N. Mitra, and Dr. J. Gillespie.

TOPICS IN SEVERAL PARTICLE DYNAMICS

Contents

CHAPTER 1

Integral Equations

1.1. Introduction

Before beginning our discussion of several particle dynamics let us review what may be called "solved problems" in theoretical physics. The list is not long. The motion of a particle of known characteristics in a fixed force field and the non-relativistic motion (but *not* the relativistic motion) of two particles interacting via a prescribed potential can be called "solved" in the sense that the trajectories may be calculated with arbitrary precision. As we shall note in more detail later, Mitra has shown that the quantum mechanical motion of three non-relativistic particles interacting via *factorable potentials* can be reduced to a form not more complicated than that of the two-body problem.

If we relax our requirements for a "solution," the above short list can be extended. The celebrated Ursell–Mayer cluster expansion for a classical gas provides a systematic method (via an infinite series of terms) for calculating the equation of state over a limited domain of temperatures and densities. A similar cluster expansion in quantum mechanics for systems of many particles was suggested by Brueckner[1] and has been developed in detail.[2,3,4] The corresponding cluster expansion in quantum statistical mechanics has been formulated by Bloch and DeDominicis.[5] Related treatments of the many-body problem using Green's functions and

[1] K. A. Brueckner, *The Many-Body Problem* (John Wiley & Sons, Inc., New York, 1959). K. A. Brueckner and J. L. Gammel, Phys. Rev. **109,** 1023 (1958).
[2] J. Goldstone, Proc. Roy. Soc. (London) **A239,** 267 (1957).
[3] N. Hugenholtz, Physica **23,** 481 (1957).
[4] W. B. Riesenfeld and K. M. Watson, Phys. Rev. **104,** 492 (1956).
[5] C. Bloch and C. DeDominicis, Nucl. Phys. **7,** 459 (1958); **10,** 181 (1959).

integral equations have been given by Martin and Schwinger,[6] Galitskii and Migdal,[7] and Weinberg.[8,9] The extension of cluster expansions to non-equilibrium phenomena has been initiated by Kubo,[10] Montroll and Ward,[11] and Prigogine,[12] among others.

The cluster expansions referred to above represent (in general) formal, rather than practical, solutions to the many-body problem. The reason for this is that the successive approximations involve solutions to the two-body problem, the three-body problem, the four-body problem, etc. Therefore, it is only to the extent that the several-body problems can be solved that practical progress can be made with the many-body problems of statistical mechanics, and atomic and nuclear physics.

It is with techniques directed toward the solution of several-body interactions that we shall be primarily concerned here.[13]

1.2. Some Integral Equations Occurring in Quantum Mechanics

We consider a physical system which may be described by a Hamiltonian H and suppose that H can be decomposed into an "unperturbed part" K and a "perturbation" V:

$$H = K + V. \tag{1.1}$$

In practice, K is supposed to be so simple that a complete set of its eigenfunctions can be explicitly exhibited. If we let E designate a complex variable, the Green's functions for H and K are, respectively,

$$G(E) = \frac{1}{E - H}, \qquad G_0(E) = \frac{1}{E - K}. \tag{1.2}$$

[6] P. C. Martin and J. Schwinger, Phys. Rev. **115,** 1342 (1959).

[7] V. M. Galitskii and A. B. Midgal, Zh. Experim. i Teor. Fiz. **34,** 139 (1958) [English transl. Soviet Phys.—JEPT **7,** 96 (1958)].

[8] S. Weinberg, Phys. Rev. **133,** B232 (1964).

[9] These techniques are reviewed in L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962).

[10] R. Kubo, J. Phys. Soc. Japan **12,** 570 (1957).

[11] E. Montroll and J. Ward, Physica **25,** 423 (1959).

[12] I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Interscience Publishers, Inc., New York, 1962).

[13] We might add to our extended list of solved problems that of the scattering of a particle by a "weakly bound" composite system, as discussed, for example, in M. L. Goldberger and K. M. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964).

G and G_0 are related by an integral equation of the Lippmann–Schwinger form[14]

$$\begin{aligned} G(E) &= G_0(E) + G_0(E)VG(E) \\ &= G_0(E) + G(E)VG_0(E). \end{aligned} \tag{1.3}$$

The *scattering matrix* $T(E)$ may be obtained from G by using the equation

$$G(E) = G_0(E) + G_0(E)T(E)G_0(E). \tag{1.4}$$

The wave function ψ_a^+ describing scattering from an initial state χ_a, such that $K\chi_a = E_a\chi_a$, can also be expressed in terms of G[15]:

$$\psi_a^+ = \lim_{\eta \to 0(+)} [1 + G(E_a + i\eta)V]\chi_a \tag{1.5}$$

The most familiar application of the above is to the calculation of the scattering cross section. For scattering from an initial state χ_a to a final state χ_b we form the matrix element

$$T_{ba} = \lim_{\eta \to 0(+)} (\chi_b, T(E_a + i\eta)\chi_a) \tag{1.6}$$

and obtain the scattering cross section in the form[16]

$$d\sigma(b \leftarrow a) = \sum_b \frac{(2\pi)^4}{v_{\text{rel}}} \delta(\mathbf{P}_b - \mathbf{P}_a)\delta(E_b - E_a)\,|T_{ba}|^2. \tag{1.7}$$

Here the sum on b runs over those final states constituting a measurement of $d\sigma$, v_{rel} is the relative velocity of the (two) colliding particles in state a, and $\mathbf{P}_b$ and $\mathbf{P}_a$ are the respective total momenta in states b and a.

Stationary state perturbation theory may also be developed in terms of the Green's function. Let the system under consideration be supposed confined to a finite volume, then the eigenvalue spectrum of H is discrete and let $K\chi_a = E_a\chi_a$, $H\psi_\lambda = E_\lambda\psi_\lambda$. Now, the poles of $(\chi_a, G(E)\chi_a)$, as a function of E, give the eigenvalues E_λ. Using Eqs. (1.3) and (1.4), we can express E_λ as[4,13]

$$E_\lambda = E_a + (\chi_a, T(E_\lambda)\chi_a). \tag{1.8}$$

[14] Equation (1.3) and similar equations may be derived on using the operator identities

$$\frac{1}{A} - \frac{1}{B} = \frac{1}{A}(B - A)\frac{1}{B} = \frac{1}{B}(B - A)\frac{1}{A},$$

where A and B are two operators possessing inverses.

[15] The relations (1.1), . . . , (1.5) are familiar in scattering theory. See, for example, Ref. 13 for a discussion of these.

[16] See, for example, Ref. 13, p. 92. It is supposed that the δ-function expressing conservation of momentum has been factored out of Eq. (1.6). See also Secs. 2.1 and 4.1.

The partition function of the canonical ensemble may also be obtained from G. That is, the partition function is

$$Z = \mathrm{Tr} \int_C dE\, e^{-\beta E} G(E), \tag{1.9}$$

with an appropriate choice for the contour C and β^{-1} the temperature.[17,18]

1.3. Mathematical Digression

The integral equations (1.3) may be written in the form

$$\begin{aligned} G(E) &= G_0(E) + \kappa(E) G(E) \\ &= G_0(E) + G(E)\kappa_t(E), \end{aligned} \tag{1.10}$$

where the *kernel* κ *is*

$$\kappa(E) \equiv G_0(E) V$$

and[19]

$$\kappa_t(E) = V G_0(E) = T_{\mathrm{T}} \kappa^{\dagger} T_{\mathrm{T}},$$

where T_{T} is the time reversal operator.[20] For a discussion of the properties of these equations it is convenient to generalize them. We write

$$G(E, \lambda) = G_0(E) + \lambda \kappa(E) G(E, \lambda), \tag{1.11}$$

where λ is a complex parameter. Clearly for $\lambda = 1$, $G(E, \lambda) = G(E)$, the "physical Green's function." Next we write

$$G(E, \lambda) \equiv \{1 + \lambda F(E, \lambda)\} G_0(E) \tag{1.12}$$

and substitute this into Eq. (1.11) to obtain

$$F(E, \lambda) = \kappa(E) + \lambda \kappa(E) F(E, \lambda). \tag{1.13}$$

Equation (1.13) is called the *resolvent equation* of κ and $F(E, \lambda)$ the *resolvent kernel.* The "physical" resolvent kernel $F(E)$ is obtained from this on setting $\lambda = 1$. It is evident from Eqs. (1.12) and (1.4) that if we can obtain $F(E, \lambda)$, then we can immediately calculate the physical properties of the system being studied.

It is beyond our present scope to discuss the mathematical theory of Eq. (1.13) in any detail. [For a more detailed discussion the reader is

[17] By "Tr [. . .]" we mean "trace of the matrix [. . .]."
[18] K. M. Watson, Phys. Rev. **103**, 489 (1956).
[19] The superscript dagger indicates an adjoint, or Hermitian conjugate, operator.
[20] The integral equation for the scattering matrix is $T(E) = V + \kappa_t(E) T(E)$.

referred to Ref. 21, 22, and 23. An excellent summary has been given by Weinberg,[24] on whose discussion we rely heavily here. A discussion of the Fredholm method is given in the Appendix.] Instead, we shall largely just quote those properties having a direct bearing on our later considerations.

The kernel $\kappa(E)$ can be represented as a matrix $\langle \mathscr{E}' | \kappa(E) | \mathscr{E} \rangle$, expressed in terms of a complete set $\mathscr{E}$ of variables describing the physical system. If

$$\tau(E) \equiv \mathrm{Tr}\,[\kappa(E)\kappa^{\dagger}(E)]$$

$$= \int |\langle \mathscr{E}' | \kappa(E) | \mathscr{E} \rangle|^2 \, d\mathscr{E}' \, d\mathscr{E} < \infty, \tag{1.14}$$

κ is said to be an $\mathscr{L}^2$ kernel (sometimes also called a Schmidt operator). For $\mathscr{L}^2$ kernels a detailed theory of the solutions of Eq. (1.13) is available.[23] A detailed theory is available also for a more general kernel, called a *compact kernel.*[21] To see what this means, we imagine that normalized wave packet states $\Psi_\alpha(\mathscr{E})$, $\alpha = 1, 2, \ldots$, are formed from some complete set of wave functions in the Hilbert space of state vectors of the physical system:

$$\|\Psi_\alpha\| \equiv [(\Psi_\alpha, \Psi_\alpha)]^{1/2} = 1. \tag{1.15}$$

The kernel $\kappa(E)$ is *compact* if for any infinite set of the Ψ_α the set

$$\kappa\Psi_\alpha \equiv \int \langle \mathscr{E} | \kappa(E) | \mathscr{E}' \rangle \, \Psi_\alpha(\mathscr{E}') \, d\mathscr{E}'$$

contains a subset converging to a limit.[25] Weinberg[24] has summarized useful properties of Eq. (1.13) for *compact* kernels, some of which we repeat here:

1. If κ is compact, it is *bounded* in the sense that all $\|\kappa\Psi_\alpha\|$ are less than some fixed number (we recall the condition that $\|\Psi_\alpha\| = 1$);

2. If the condition (1.14) is satisfied, κ is compact;

3. If it is compact, κ can be represented to arbitrary accuracy by a kernel of *finite rank*, that is,

$$\langle \mathscr{E}' | \kappa | \mathscr{E} \rangle \cong \sum_{i=1}^{p} \chi_i(\mathscr{E}') \bar{\chi}_i^{\dagger}(\mathscr{E}), \tag{1.16}$$

where χ_i and $\bar{\chi}_i$ are two sets of states each of finite norm;

[21] F. Riesz and B. Sz.-Nagy, *Functional Analysis* (Frederich Ungar Publishing Co., New York, 1955).

[22] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, Inc., New York, 1962).

[23] F. Smithies, *Integral Equations* (Cambridge University Press, New York, 1958).

[24] S. Weinberg, Phys. Rev. **130,** 776 (1963); **131,** 440 (1963).

[25] The term *completely continuous*, rather than *compact*, is used in Refs. 21 and 24. This is evidently a generalization of a *continuous* kernel; that is, a kernel $\langle \mathscr{E} | \kappa(E) | \mathscr{E}' \rangle$ which is a *continuous* function of its variable sets $\mathscr{E}$ and $\mathscr{E}'$.

4. The resolvent operator $F(E, \lambda)$ is said to be bounded if $\|F\Psi_\alpha\|$ is finite (in the sense defined by property 1 above) for all of our normalized wave packet states Ψ_α. It is said to be analytic in λ if all matrix elements $(\Psi_\beta, F\Psi_\alpha)$ are analytic functions of λ. If F is bounded in some domain of λ, it can be shown to be analytic in λ. A point λ at which F is bounded and analytic is said to belong to the *resolvent set* of κ. Points λ at which F is not both bounded and analytic are called the "spectrum" of κ.

For a compact (or $\mathscr{L}^2$) kernel the spectrum of κ forms a discrete set λ_σ ($\sigma = 1, 2, \ldots$), with no finite limit point, called the *point spectrum.* Corresponding to each λ_σ there is a normalizable state vector Φ_σ such that

$$\kappa\Phi_\sigma = \frac{1}{\lambda_\sigma}\Phi_\sigma, \tag{1.17a}$$

or, equivalently,

$$\lambda_\sigma V\Phi_\sigma = (E - K)\Phi_\sigma. \tag{1.17b}$$

For any $\lambda_\sigma = 1$, Eq. (1.17b) is the Schrödinger equation for a bound state and the "physical" resolvent kernel $F(E)$ is singular.

Kernels which are not compact may have in addition to a point spectrum what is called a "continuous spectrum."[24]

It is in general not easy to determine if a given kernel κ is compact, but is usually straightforward to determine if it is an $\mathscr{L}^2$ kernel [that is, satisfies (1.14)]. In quantum mechanical theory the relatively simpler theory[23] of $\mathscr{L}^2$ kernels is ordinarily used when applicable.

1.4. Some Techniques for Solving Integral Equations

By successive substitution of the right-hand side of Eq. (1.13) for F on the right, we obtain the Born (sometimes called the Neumann) series

$$F(E, \lambda) = \kappa + \lambda\kappa^2 + \lambda^2\kappa^3 + \cdots. \tag{1.18}$$

If κ is compact this series converges for $|\lambda| < |\lambda_0|$, where $|\lambda_0|$ is the smallest of the $|\lambda_\sigma|$ obtained from Eq. (1.17). A sufficient condition to establish the convergence of the series (1.18) is that[26,27]

$$|\lambda|^2\tau(E) < 1, \tag{1.19}$$

where $\tau(E)$ is defined by Eq. (1.14).

[26] See, for example, Ref. 23, p. 29.

[27] M. Scadron, S. Weinberg, and J. Wright, Phys. Rev. **135,** B202 (1964), have shown that in scattering theory this often provides a practical test for convergence.

An important formal method for discussing solutions to Eq. (1.13) for $\mathscr{L}^2$ kernels is based on the Fredholm theory. To describe this, we choose an adequate approximation to κ of the form (1.16), so Eq. (1.13) reads

$$\langle \mathscr{E}' | F | \mathscr{E} \rangle = \sum_{i=1}^{p} \chi_i(\mathscr{E}') \left\{ \bar{\chi}_i^\dagger(\mathscr{E}) + \lambda \int \bar{\chi}_i^\dagger(\mathscr{E}'') \langle \mathscr{E}'' | F | \mathscr{E} \rangle \, d\mathscr{E}'' \right\}.$$

On defining

$$\Gamma_i(\mathscr{E}) \equiv \int \bar{\chi}_i^\dagger(\mathscr{E}'') \langle \mathscr{E}'' | F | \mathscr{E} \rangle \, d\mathscr{E}'',$$

we may write Eq. (1.13) in the form

$$\langle \mathscr{E}' | F | \mathscr{E} \rangle = \langle \mathscr{E}' | \kappa | \mathscr{E} \rangle + \lambda \sum_{i=1}^{p} \chi_i(\mathscr{E}') \Gamma_i(\mathscr{E}). \tag{1.20}$$

Operating from the left with $\bar{\chi}_j^\dagger(\mathscr{E}')$ gives

$$\Gamma_j(\mathscr{E}) = \sum_{i=1}^{p} [\kappa_{ji} \bar{\chi}_i^\dagger(\mathscr{E}) + \lambda \kappa_{ji} \Gamma_i(\mathscr{E})],$$

where

$$\kappa_{ji} \equiv \int d\mathscr{E} \bar{\chi}_j^\dagger(\mathscr{E}) \chi_i(\mathscr{E}).$$

Next, we write

$$\Gamma_i(\mathscr{E}) = \sum_{s=1}^{p} F_{is} \bar{\chi}_s^\dagger(\mathscr{E}) \tag{1.21}$$

to obtain

$$F_{js} = \kappa_{js} + \lambda \sum_i \kappa_{ji} F_{is}. \tag{1.22}$$

This has the form of Eq. (1.13), but with finite matrices. Equation (1.21) has the solution

$$F_{is} = \sum_j \frac{N_{ij}}{D} \kappa_{js}, \tag{1.23}$$

where

$$D(E, \lambda) = \det a_{ij}, \tag{1.24}$$

with $a_{ij} \equiv \delta_{ij} - \lambda \kappa_{ij}$, and

$$N_{ij} = \frac{\partial D}{\partial a_{ji}}. \tag{1.25}$$

If the solution (1.23) is inserted into Eq. (1.21) and the result into Eq. (1.20), we obtain $F(E, \lambda)$. The solution exists when the Fredholm determinant $D(E, \lambda) \neq 0$ and may, in principle, be made to approximate

as accurately as desired the solution to Eq. (1.13) by choosing a sufficiently accurate representation (1.16).

A convenient notation for the Fredholm solution to the exact equation

$$[1 - \lambda\kappa(E)]F(E, \lambda) = \kappa(E)$$

[this is Eq. (1.13)] is

$$F(E, \lambda) = \frac{N(E, \lambda)}{D(E, \lambda)}\kappa(E), \tag{1.26}$$

where the Fredholm determinant is[28]

$$D(E, \lambda) = \det [1 - \lambda\kappa(E)] \tag{1.27}$$

and N is an appropriate operator. For $\lambda = 1$, we write Eq. (1.26) simply as

$$F(E) = \frac{N(E)}{D(E)}\kappa(E). \tag{1.28}$$

When κ is $\mathscr{L}^2$, $N(E)$ and $D(E)$ are analytic functions of E in any domain in which κ is analytic.

This follows from the facts that each term of the Fredholm series is analytic in E and the series for N and D are uniformly convergent. Actually, $F(E)$ is meromorphic for any compact, analytic $\kappa(E)$. It is also interesting to point out that the residue of $F(E)$ at a pole due to a zero of $D(E)$ is an operator of finite rank.

As we shall see in Chapter 3, given the Fredholm determinant $D(E)$, one can construct the physical scattering matrix T for scattering involving only two-particle channels.

Weinberg[24] has suggested a method combining the Born and Fredholm treatments, which he calls the *quasi-particle* method. When the series (1.18) fails to converge for the "physical" value $\lambda = 1$, we have seen that this results from there being one or more eigenvalues λ_σ such that $|\lambda_\sigma| < 1$. Weinberg's proposal is to modify the kernel in such a way that there are no λ_σ's of magnitude less than unity. To do this, he writes [instead of Eq. (1.16)] for a compact kernel κ

$$\langle \mathscr{E}' | \kappa | \mathscr{E} \rangle = \langle \mathscr{E}' | \kappa_1 | \mathscr{E} \rangle + \sum_{i=1}^{p} \omega_i(\mathscr{E}')\bar{\omega}_i^{\dagger}(\mathscr{E}), \tag{1.29}$$

[28] Equation (1.27) is defined in the usual sense if κ has a matrix representation with discrete indices. When κ has continuously variable indices the determinant is often defined by letting these represent the limit of a set of discrete indices. Equation (A.14) provides another sometimes useful definition of det $[1 - \lambda\kappa]$. The Fredholm formulae of the Appendix provide yet other ways of defining this quantity. More general definitions are given, for example, in Chapter VI of Ref. 23.