Scattering theory

Dmitry A. Konovalov
Discipline of Information Technology, School of Business, James Cook University, Townsville, Queensland 4811, Australia

Igor Bray
ARC Centre for Antimatter-Matter Studies, Curtin University, GPO Box U1987, Perth, Western Australia 6845, Australia
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I. INTRODUCTION

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II. THEORY

A. Potential Scattering

After the partial-wave expansion and retaining only the s-wave terms ($l = 0$), the potential scattering problem is reduced [1, 2] to solving the radial Schrödinger equation

$$(H - E)\Psi(k, r) = 0, \quad E = k^2/2, \tag{1}$$

$$\Psi(k, r \to \infty) \sim \sin(kr + \delta_0), \quad \Psi(k, r \to 0) = 0, \tag{2}$$

$$H = K + V(r), \quad K = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2}, \tag{3}$$

where δ_0 is the s-wave phase shift and E is the total energy of the system.

$$\langle \xi_m | \xi_{m'} \rangle = \delta_{mm'}, \quad m, m' = 0, 1, ..., \infty, \tag{4}$$

$$\langle \Psi_i | H | \Psi_j \rangle = E_i \delta_{ij}, \quad \langle \Psi_i | \Psi_j \rangle = \delta_{ij}. \tag{5}$$

$$\Psi_i^{\mathrm{JM}}(r) = \sum_{m=0}^{N-1} A_{im} \phi_m(r), \tag{6}$$

$$\Psi_i^{\mathrm{KB}}(r) = \sum_{m=0}^{N-1} B_{im} \xi_m(r), \tag{7}$$

$$\hat{P}_{\mathrm{KB}} = \sum_{m=0}^{N-1} |\xi_m\rangle\langle\xi_m|. \tag{8}$$

To help explain the logic, the new method (denoted KB) is presented together with the original JM method,

$$\Psi_{\mathrm{JM}}(r) = \sum_j \Psi_j^{\mathrm{JM}}(r) a_j + \sum_{p=N}^{\infty} \phi_p(r) f_p, \tag{9}$$

$$\Psi_{\mathrm{KB}}(r) = \sum_j \Psi_j^{\mathrm{KB}}(r) b_j + (1 - \hat{P}_{\mathrm{KB}}) \sin(kr + \delta_0), \tag{10}$$

$$\Psi_{\mathrm{KB}}^{+}(r) = \sum_j \Psi_j^{\mathrm{KB}}(r) b_j + (1 - \hat{P}_{\mathrm{KB}}) \Delta_0 \exp(ikr), \tag{11}$$

where $\Delta_0 = \exp(i\delta_0)$, a_m are the *inner*-space expansion coefficients describing the electron's interaction with $V(r)$, and $R = \tan\delta$ is the s-term of the reactance matrix (also known as the K matrix [2]). The second sum in (**??**) is the *outer*-space part describing a free moving electron in terms of the regular or sine-like (s_p -coefficients) and irregular or cosine-like (c_p -coefficients) solutions of

For the potential scattering, such orthonormal basis could be constructed from the diagonalization of the system's Hamiltonian,

$$\sum_{p=0}^{\infty} J_{np} s_p = 0, \quad \sum_{p=0}^{\infty} J_{np} c_p = w\delta_{n,0}, \tag{12}$$

with a uniquely defined constant w. The unknown a_m and R are found by simultaneously solving

$$\langle \chi_n | H - E | \Psi^N \rangle = 0, \quad n < N, \tag{13}$$

$$\langle \phi_n | H - E | \Psi^N \rangle = 0, \quad n \geq N. \tag{14}$$

Note that the equations (12) are central to the JM formalism as they could be solved analytically for some types of the basis functions [3]. To take advantage of the analytical solutions for s_n and c_n, the representation of $V(r)$ in the chosen basis is truncated to an $N \times N$ matrix by retaining only the inner functional-space contributions,

$$V_{nm} \approx V_{nm}^N = \begin{cases} \langle \phi_n | V | \phi_m \rangle & \text{if } n, m < N \\ 0 & \text{otherwise,} \end{cases} \tag{15}$$

obtaining

$$\langle\chi_n|H-E|\phi_p\rangle \approx \langle\chi_n|K-E|\phi_p\rangle, \quad n<N,\ p\geq N, \tag{16}$$

$$\langle\phi_p|H-E|\phi_{p'}\rangle \approx J_{pp'}, \quad p,p'\geq N. \tag{17}$$

By this neglecting V_{nm} in the outer functional space, Eqs. (13) and (14) are reduced to the following three cases

$$(e_n-E)a_n = -D_{n,N-1}J_{N-1,N}f_N, \quad n<N, \tag{18}$$

$$\sum_{m=0}^{N-1} D_{m,N-1}a_m = f_{N-1}, \quad n=N, \tag{19}$$

$$\sum_{p=N}^{\infty} J_{np}f_p = 0, \quad n>N, \tag{20}$$

where (20) is automatically satisfied via (12) and

$$J_{NN}f_N + J_{N,N+1}f_{N+1} = -J_{N,N-1}f_{N-1} \tag{21}$$

was used in (19).

Note that while the original JM formulation used $\phi_m(r)$ instead of $\chi_m(r)$ in (**??**), the final expression for R remains the same completing the JM treatment of the potential scattering,

$$R = -(WCJC)^{-1}(WSJS), \tag{22}$$

where the s-wave partial S-matrix and elastic cross section are given by

$$S_{00} = (1+\mathrm{i}R)(1-\mathrm{i}R)^{-1}, \tag{23}$$

$$\sigma_{00} = \frac{\pi}{k^2}|S_{00}-1|^2, \tag{24}$$

respectively, and where

$$(WSJS) = Ws_N J_{N,N-1} + s_{N-1}, \tag{25}$$

$$(WCJC) = Wc_N J_{N,N-1} + c_{N-1}, \tag{26}$$

$$W = \sum_{m=0}^{N-1} \frac{D^2_{m,N-1}}{e_m - E}. \tag{27}$$

III. CONCLUSIONS

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Acknowledgments

[1] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics (Non-relativistic theory)*, vol. 3 of *Course of theoretical physics* (Pergamon press, Oxford, 1985), 3rd ed.
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[3] H. A. Yamani, A. D. Alhaidari, and M. S. Abdelmonem, Phys. Rev. A **64**, 042703 (2001).