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Research Note

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# Ellipsoidal Microhydrodynamics without Elliptic Integrals and How To Get There Using Linear Operator Theory: A Note on Weighted Inner Products

Sangtae Kim*

School of Chemical Engineering, Purdue University, West Lafayette, Indiana 47907, United States

**ABSTRACT:** In this research note we revisit the topic of microhydrodynamics of an ellipsoid in rigid body motion to arrive at the final resolution of a 140-year-old "mystery" that was featured in the dedication paper on the same topic in the Doraiswami Ramkrishna Festschrift. There, the initial focus was on the role of the theory of self-adjoint operators as the framework for proving that the surface tractions on a sphere had to be a constant multiple of the same rigid body motions of the boundary conditions. The ellipsoid was then considered as a simple example to illustrate the loss of this behavior for nonspherical particles. That goal was accomplished because for an ellipsoid, $\mathbf{n}\cdot\boldsymbol{x}$, the dot product of the surface normal $\mathbf{n}$ and the point $\boldsymbol{x}$ on the ellipsoid surface, is the required nonconstant multiplier. The simplicity of this result is striking and has been noticed throughout its history with a number of authors remarking on the lengthy algebraic manipulations required to prove this simple result. In keeping with the theme of the Doraiswami Ramkrishna Festschrift, this note presents a short and simple proof that highlights the importance of the choice of the inner product, that is, the definition of the metric. The introduction of $\boldsymbol{n}\cdot\boldsymbol{x} = w(x)$ as a so-called *weight function* in the definition of the *weighted* inner product, as in $\langle f, g\rangle_w = \int f(s)g(s)w(s)\mathrm{d}s$ over the appropriate metric space transforms the double layer operator (DLO) into a *self-adjoint* operator. From this it follows that the eigenfunctions of the adjoint with respect to the nonweighted inner product are $w$ times the DLO eigenfunctions. Thus, the simplification noted in the companion paper is true for all eigenvalues and eigenfunctions of the double layer operator and not just the eigenvalue of $-1$ and its associated eigenfunction $\boldsymbol{v}^{\mathrm{RBM}}$. These insights open the door to significant opportunities in the computational analysis of ellipsoidal particles in nanoparticle technology including topics such as perturbation methods for inertial and non-Newtonian effects, as we now have ready access to the spectral decomposition and biorthogonal expansions for the double layer operator.

## INTRODUCTION

In this research note we revisit the topic of microhydrodynamics of an ellipsoidal particle in rigid body motion to arrive at the final resolution of a 140-year-old "mystery" (with key plot developments in 1876, 1892, and 1964) that surfaced in the dedication paper on the same topic in the Doraiswami Ramkrishna Festschrift. In that companion paper,[1] the initial focus was on the role of the theory of self-adjoint operators as the framework for proving that the surface tractions on a sphere had to be a constant times the same rigid body motions of the boundary conditions. The ellipsoid was then considered as a simple example to illustrate the loss of this behavior for nonspherical particles. That goal was accomplished because for an ellipsoid, the surface tractions are $\boldsymbol{n}\cdot\boldsymbol{x}$ times a rigid body motion where the dot product of the surface normal $\boldsymbol{n}$ and the point $\boldsymbol{x}$ on the surface of the ellipsoid is the required nonconstant function. The simplicity of this result is striking and has been noticed throughout its history with a number of authors remarking on the simple but lengthy algebraic manipulations required to prove this result. (For example, the author used five pages of neatly written notes to verify the results for a translating ellipsoid).

In keeping with the theme of the Doraiswami Ramkrishna Festschrift, this note presents a simple proof that highlights the importance of the choice of the inner product. The introduction of $\boldsymbol{n}\cdot\boldsymbol{x} = w(\boldsymbol{x})$ as a so-called *weight function* in the definition of the *weighted* inner product, as in $\langle f, g\rangle_w = \int f(s)g(s)w(s)\mathrm{d}s$ over the appropriate metric space, leads to the conclusion that for an ellipsoid, the double layer operator $\mathcal{K}$ is *self-adjoint* with respect to this weighted inner product; that is, $\mathcal{K} = \mathcal{K}^{*w}$. Thus, if $\boldsymbol{v}$ is an eigenfunction of $\mathcal{K}$ then it is also an eigenfunction of $\mathcal{K}^{*w}$, which in turn implies that $w\boldsymbol{v}$ is the associated eigenfunction of $\mathcal{K}^*$ (the adjoint with respect to the standard, nonweighted inner product). This result is true for all eigenvalues and eigenfunctions of the double layer operator including the all-important eigenvalue of $-1$ and its six associated eigenfunctions $\boldsymbol{v}^{\mathrm{RBM}}$ corresponding to the six "basis" rigid body motions. These insights open the door to significant opportunities in the computational analysis of ellipsoidal particles in nanoparticle technology including topics such as perturbation solutions for inertial and non-Newtonian effects as we now have ready access to the spectral decomposition and biorthogonal expansion for the double layer operator.

## RESULTS AND DISCUSSION

**Integral Operators and Weighted Inner Products.** The required background information on microhydrodynamics is described in the companion paper[1] and is not repeated here. As

Special Issue: Doraiswami Ramkrishna Festschrift

Received: July 4, 2015
Accepted: August 5, 2015
Published: August 5, 2015

  

DOI: 10.1021/acs.iecr.5b02431
Ind. Eng. Chem. Res. 2015, 54, 10549−10551

in the companion paper, we follow the notation of Kim and Karrila[2] for the double layer operator $\mathcal{K}$ with a kernel given by

$$K(\boldsymbol{x}, \boldsymbol{\xi}) = \frac{3}{2\pi}\boldsymbol{n}(\boldsymbol{\xi})\cdot\frac{(\boldsymbol{x}-\boldsymbol{\xi})(\boldsymbol{x}-\boldsymbol{\xi})(\boldsymbol{x}-\boldsymbol{\xi})}{|\boldsymbol{x}-\boldsymbol{\xi}|^5} \tag{1}$$

and considering first the standard (unweighted) inner product we have the kernel for its adjoint as $K^*_{ij}(\boldsymbol{x}, \boldsymbol{\xi}) = K_{ji}(\boldsymbol{\xi}, \boldsymbol{x})$ . The book by Professor Ramkrishna[3] provides an instructive reminder that this expression for the kernel of the adjoint follows from the definition and requirement that $\langle\mathcal{K}(\boldsymbol{v}), \boldsymbol{t}\rangle = \langle\boldsymbol{v}, \mathcal{K}^*(\boldsymbol{t})\rangle$ which when expressed in expanded form as the actual integrals,

$$\begin{aligned}\langle\mathcal{K}(\boldsymbol{v}), \boldsymbol{t}\rangle &= \int_S\int_S K_{ij}(\boldsymbol{x}, \boldsymbol{\xi})\boldsymbol{v}_j(\boldsymbol{\xi})\boldsymbol{t}_i(\boldsymbol{x})\,\mathrm{d}S(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{x})\\ &= \int_S\int_S K_{ji}(\boldsymbol{\xi}, \boldsymbol{x})\boldsymbol{v}_i(\boldsymbol{x})\boldsymbol{t}_j(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{x})\\ \langle\boldsymbol{v}, \mathcal{K}^*(\boldsymbol{t})\rangle &= \int_S\int_S K^*_{ij}(\boldsymbol{x}, \boldsymbol{\xi})\boldsymbol{t}_j(\boldsymbol{\xi})\boldsymbol{v}_i(\boldsymbol{x})\,\mathrm{d}S(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{x})\end{aligned}$$

align the kernels for ease of identification (after renaming the dummy variables and indices and interchanging the order of integrations on the surface of the particle).

We now consider the same procedure but with the weighted inner product,

$$\langle\boldsymbol{v}, \boldsymbol{t}\rangle_w = \int_S \boldsymbol{v}(\boldsymbol{\xi})\boldsymbol{t}(\boldsymbol{\xi})w(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{\xi}) \tag{2}$$

where the key requirement for the weight function is that it must be positive everywhere on the surface; that is, $w(\boldsymbol{\xi}) > 0$ on $S$. Now we have for the same alignment procedure,

$$\begin{aligned}\langle\mathcal{K}(\boldsymbol{v}), \boldsymbol{t}\rangle_w &= \int_S\int_S K_{ij}(\boldsymbol{x}, \boldsymbol{\xi})\boldsymbol{v}_j(\boldsymbol{\xi})\boldsymbol{t}_i(\boldsymbol{x})w(\boldsymbol{x})\,\mathrm{d}S(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{x})\\ &= \int_S\int_S K_{ji}(\boldsymbol{\xi}, \boldsymbol{x})\boldsymbol{v}_i(\boldsymbol{x})\boldsymbol{t}_j(\boldsymbol{\xi})w(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{x})\\ \langle\boldsymbol{v}, \mathcal{K}^{*w}(\boldsymbol{t})\rangle_w &= \int_S\int_S K^{*w}_{ij}(\boldsymbol{x}, \boldsymbol{\xi})\boldsymbol{t}_j(\boldsymbol{\xi})\boldsymbol{v}_i(\boldsymbol{x})w(\boldsymbol{x})\,\mathrm{d}S(\boldsymbol{\xi})\\ &\qquad \mathrm{d}S(\boldsymbol{x})\end{aligned}$$

and the result

$$K^{*w}_{ij}(\boldsymbol{x}, \boldsymbol{\xi}) = K_{ji}(\boldsymbol{\xi}, \boldsymbol{x})\frac{w(\boldsymbol{\xi})}{w(\boldsymbol{x})} = K^*_{ij}(\boldsymbol{x}, \boldsymbol{\xi})\frac{w(\boldsymbol{\xi})}{w(\boldsymbol{x})} \tag{3}$$

which highlights the role of the inner product in the definition of the adjoint.

**The Ellipsoid and Its Surface Normal.** We now consider an ellipsoid whose surface is defined by the equation

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = \frac{x_ix_i}{a_i^2} = 1 \tag{4}$$

with different values for the semiaxes $a = a_1 > b = a_2 > c = a_3$. The repeated index $i$ imply summation from 1 to 3 by the usual Einstein summation convention.

The surface normal $\boldsymbol{n}(\boldsymbol{x})$ at the point $\boldsymbol{x}$ or coordinates $(x_1, x_2, x_3) = (x, y, z)$ satisfies a useful relation which in index notation is given by

$$\boldsymbol{n}_i(\boldsymbol{x}) = \frac{x_i}{a_i^2}(\boldsymbol{n}\cdot\boldsymbol{x}), \qquad \text{(no sum on } i\text{)} \tag{5}$$

so that the dot product that appears in the definition of the kernel in eq 1 may be manipulated as follows

$$\begin{aligned}&K^{*w}_{ij}(\boldsymbol{x}, \boldsymbol{\xi})\\ &= K_{ji}(\boldsymbol{\xi}, \boldsymbol{x})\frac{w(\boldsymbol{\xi})}{w(\boldsymbol{x})}\\ &= \frac{3}{2\pi}\boldsymbol{n}(\boldsymbol{x})\cdot(\boldsymbol{\xi}-\boldsymbol{x})\frac{(x_i-\xi_i)(x_j-\xi_j)}{|\boldsymbol{x}-\boldsymbol{\xi}|^5}\frac{w(\boldsymbol{\xi})}{w(\boldsymbol{x})}\\ &= \frac{3}{2\pi}(\boldsymbol{n}(\boldsymbol{x})\cdot\boldsymbol{x})\left[\frac{x_k\xi_k}{a_k^2} - 1\right]\frac{(x_i-\xi_i)(x_j-\xi_j)}{|\boldsymbol{x}-\boldsymbol{\xi}|^5}\frac{w(\boldsymbol{\xi})}{w(\boldsymbol{x})}\\ &= \frac{3}{2\pi}(\boldsymbol{n}(\boldsymbol{\xi})\cdot\boldsymbol{\xi})\left[\frac{x_k\xi_k}{a_k^2} - 1\right]\frac{(x_i-\xi_i)(x_j-\xi_j)}{|\boldsymbol{x}-\boldsymbol{\xi}|^5}\frac{w(\boldsymbol{\xi})}{w(\boldsymbol{x})}\\ &\quad\frac{(\boldsymbol{n}(\boldsymbol{x})\cdot\boldsymbol{x})}{(\boldsymbol{n}(\boldsymbol{\xi})\cdot\boldsymbol{\xi})}\\ &= \frac{3}{2\pi}\boldsymbol{n}(\boldsymbol{\xi})\cdot(\boldsymbol{x}-\boldsymbol{\xi})\frac{(x_i-\xi_i)(x_j-\xi_j)}{|\boldsymbol{x}-\boldsymbol{\xi}|^5}\frac{w(\boldsymbol{\xi})}{w(\boldsymbol{x})}\frac{(\boldsymbol{n}(\boldsymbol{x})\cdot\boldsymbol{x})}{(\boldsymbol{n}(\boldsymbol{\xi})\cdot\boldsymbol{\xi})}\\ &= K_{ij}(\boldsymbol{x}, \boldsymbol{\xi})\end{aligned} \tag{6}$$

where the last step is valid for all $w(\boldsymbol{x})$ that are a constant times $\boldsymbol{n}(\boldsymbol{x})\cdot\boldsymbol{x}$. For such weighting, the *double layer operator is self-adjoint with respect to the weighted inner product*. The choice $w(\boldsymbol{x}) = a^{-1}(\boldsymbol{n}\cdot\boldsymbol{x})$ is convenient because, for the degenerate case of the sphere, $w = 1$, and the "weighting" becomes latent.

We now consider the implications for the eigenspaces of $\mathcal{K}$ and its two adjoints for the ellipsoid. If $\boldsymbol{v}$ is an eigenfunction of $\mathcal{K}$, the corresponding eigenvalue−eigenfunction relationship for the two adjoint operators becomes (keeping in mind that $\mathcal{K}$ is self-adjoint with respect to the weighted inner product)

$$\begin{aligned}&\int_S K^{*w}_{ij}(\boldsymbol{x}, \boldsymbol{\xi})v_j(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{\xi})\\ &= \int_S K^*_{ij}(\boldsymbol{x}, \boldsymbol{\xi})\frac{w(\boldsymbol{\xi})}{w(\boldsymbol{x})}v_j(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{\xi})\\ &= \lambda v_i(\boldsymbol{x})\end{aligned} \tag{7}$$

or equivalently,

$$\int_S K^*_{ij}(\boldsymbol{x}, \boldsymbol{\xi})w(\boldsymbol{\xi})v_j(\boldsymbol{\xi})\,\mathrm{d}S(\boldsymbol{\xi}) = \lambda w(\boldsymbol{x})v_i(\boldsymbol{x}) \tag{8}$$

which is the standard result from linear operator theory that the (unweighted) adjoint has the eigenfunction $w\boldsymbol{v}$ if the operator is self-adjoint with respect to the weighted inner product.

We have achieved a satisfactory closure to a question raised during the long history of ellipsoidal microhydrodynamics that has been marked by the contributions of Oberbeck[4] (1874, translating ellipsoid), Edwardes[5] (1892, rotating ellipsoid), and Brenner[6] (1964, expressions for the surface tractions). In particular, as described in the companion paper, Brenner's (1964) *tour de force* can be used to deduce that the surface tractions for translation and rotation are $\boldsymbol{n}\cdot\boldsymbol{x}$ times the six canonical rigid body motions,

$$\boldsymbol{t}^{\mathrm{RBM(trans)}}(\boldsymbol{x}) = \frac{(\boldsymbol{n}\cdot\boldsymbol{x})}{4\pi abc}\boldsymbol{F} \tag{9}$$


DOI: 10.1021/acs.iecr.5b02431
*Ind. Eng. Chem. Res.* 2015, 54, 10549−10551

$$t^{RBM(\mathrm{rot})}(\boldsymbol{x}) = \frac{3(\boldsymbol{n}\cdot\boldsymbol{x})}{4\pi abc}(\mathbf{P}\cdot\boldsymbol{T}) \times \boldsymbol{x},$$

$$\boldsymbol{P} = \begin{pmatrix} (b^2 + c^2)^{-1} & 0 & 0 \\ 0 & (c^2 + a^2)^{-1} & 0 \\ 0 & 0 & (a^2 + b^2)^{-1} \end{pmatrix} \tag{10}$$

and we now recognize these surprisingly simple results as a requirement of the general theory applied to the special case for the $\lambda = -1$ eigenspace of $\mathcal{K}$.

## CONCLUSIONS

As mentioned in the companion paper, the wonderful connection between linear operators and transport phenomena highlights once again the power of mathematics in unifying the pedagogical framework for chemical engineers and the great influence of Professor Ramkrishna over the past half-century. It is especially appropriate that as we honor Professor Ramkrishna, his and the author's shared fondness for the *weighted inner product* adds a most helpful dimension to the solution of a 140-year old mystery. The author had conjectured a solution strategy based on weighted inner products almost 30 years ago during the writing of Kim and Karrila's *Microhydrodynamics*; nevertheless the formal proof as described in this note was spurred only recently by the author's current research focus on the construction of abstract metric spaces as an element of rational computer-aided drug design.

The relatively simple results for the surface traction on an ellipsoid for the RBM boundary value problem with the force or torque as the known inputs may now be generalized as follows. *The double layer operator is not self-adjoint for the ellipsoid when the standard inner product is employed, but the introduction of $(\boldsymbol{n}\cdot\boldsymbol{x})/a = w(\boldsymbol{x})$ as the weight function produces a self-adjoint operator with respect to the weighted inner product. Consequently, the eigenfunctions of $\mathcal{K}^*$ are $\boldsymbol{n}\cdot\boldsymbol{x}$ times the corresponding eigenfunctions of $\mathcal{K}$ for all eigenvalues $\lambda$.* For the sphere, $w = 1$, because we have scaled the dot product by the dimensional factor of $a$, the standard inner product is employed always. Furthermore, we note that the double layer operator for the ellipsoid has a biorthogonal expansion of the form:

$$\mathcal{K}(\bullet) = \sum_{\lambda_i} \lambda_i \psi_i \langle \psi_i, \bullet \rangle_w = \sum_{\lambda_i} \lambda_i \psi_i \langle w\psi_i, \bullet \rangle \tag{11}$$

once we construct the appropriate orthonormal basis set $\{\psi_i\}$ for the eigenspaces of $\mathcal{K}$ from the general solution of the ellipsoid as given in Kim and Karrila.[2]

For the microhydrodynamic community, this note provides a simple description of the eigenspace of the adjoint of the double layer operator, namely that they are simply $\boldsymbol{n}\cdot\boldsymbol{x}$ times the corresponding eigenfunctions of $\mathcal{K}$. These insights open the door to new opportunities in the computational analysis of ellipsoids in nanoparticle technology including topics such as perturbation solutions for inertial and non-Newtonian effects via access to the spectral decomposition and biorthogonal expansions for the double layer operator.

## AUTHOR INFORMATION


### Corresponding Author

*Tel:+1 765-494-3492. E-mail: kim55@purdue.edu.


### Notes

The authors declare no competing financial interest.

## ACKNOWLEDGMENTS

The author thanks Korea University (KU) for the opportunity to revisit ellipsoidal microhydrodynamics during a summer 2015 visit to KU as part of the KU−Purdue international alliance as sponsored by the BK-21-Plus program.

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DOI: 10.1021/acs.iecr.5b02431
*Ind. Eng. Chem. Res.* 2015, 54, 10549−10551