Properties of Index Transforms in Modeling of Nanostructures and Plasmonic Systems

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In material structures with nanometer scale curvature or dimensions electrons may be excited to oscillate in confined spaces. The consequence of such geometric confinement is of great importance in nano-optics and plasmonics. Furthermore, the geometric complexity of the probe-substrate/sample assemblies of many scanning probe microscopy experiments often pose a challenging modeling problem due to the high curvature of the probe apex or sample surface protrusions and indentations. Index transforms such as Mehler-Fock and Kontorovich-Lebedev, where integration occurs over the index of the function rather than over the argument, prove useful in solving the resulting differential equations when modeling optical or electronic response of such problems. By considering the scalar potential distribution of a charged probe in presence of a dielectric substrate, we discuss certain implications and criteria of the index transform and prove the existence and the inversion theorems for the Mehler- Fock transform of the order $m \in \mathbb{N}_0$. The probe charged to a potential V_0, measured at the apex, is modeled, in the non-contact case, as a one-sheeted hyperboloid of revolution, and in the contact case or in the limit of a very sharp probe, as a cone. Using the Mehler-Fock integral transform in the first case, and the Fourier integral transform in the second, we discuss the necessary conditions imposed on the potential distribution on the probe surface.

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I. INTRODUCTION

The complicated interaction between two bodies $\mathbf{O}_i, i = 1, 2$, shown in Fig. 1, as their relative distance is reduced beyond a few nanometers (10^{-9} meters), encompasses a wide range of forces operative at their respective length scales. Neglecting gravity, these forces are ultimately electrodynamic (Van der Waals, Casimir, Coulomb, etc.) in origin. Monitoring the dynamical attributes of $\mathbf{O_1}$, for example its oscillation eigenfrequency, such forces allow $\mathbf{O_1}$ to probe $\mathbf{O_2}$. This is the principle of operation for many scanning probe microscopes [1] (SPM), where one object $\mathbf{O_1}$ is the probe and a second $\mathbf{O_2}$ is the sample under study. In most cases, the atoms making up the apex region of a probe, and those in a volume of the sample/substrate closest to the probe constitute the engaging parts, as schematically shown in Fig. 2. The probe, typically a small (a few nanometers) sized sharp material domain interacts with a the sample/substrate surface under study, see Fig. 3. SPMs can be considered an extension of human visual range, as visual inspection of the atomic fabrics of our physical environment was not necessary for survival of human species rendering our eyesight limited to just below millimeter range. The probing capability of most SPMs can therefore, albeit somewhat metaphorically, be compared to the tips of the fingers ($\mathbf{O_1}$) of a blind, "probing" and sensing the topography of a Braille script ($\mathbf{O_2}$).

In situations where the electrodynamics of the interacting bodies $\mathbf{O}_i, i \in \mathbb{N}$ can be approximated by quasi-statics, significant simplification can be achieved due to the negligence of retardation in sub-wavelength regions, that is, regions of the system with a dimension smaller than the interacting photon wavelength [2]. Here, a closely related example, classically experimented with by Newton in

1665, and found in many SPM work, is the quantum mechanical phenomenon of photon tunneling between the two prisms $\mathbf{O_1}$ and $\mathbf{O_2}$. As shown in Fig. 4, for photons of wavelength λ, when $|\mathbf{r_1} - \mathbf{r_2}| \propto \lambda$, tunneling commences prior to full transmission of light at $|\mathbf{r_1} - \mathbf{r_2}| \to 0$ corresponding to the disappearance of the gap. The objects in Fig. 1-Fig. 4 are depicted as finite, but in many cases one or several dimensions of the system can be large and may be considered as infinite, for example the dimensions in the x and z directions with respect to the gap size of Fig. 4. When satisfying the boundary conditions for such problems, the encountered divergent or slowly converging integrals associated with an infinite dimension of the modeling geometry can raise major numerical issues. Thus, for any realistic model, careful truncation criteria are required in order that the finiteness of the probe size, and it's experimentally imposed potential (boundary conditions) be accounted for.

An example of such a modeling geometry is shown in the cartesian tunneling system shown in Fig. 5. Other examples, such as the metal coated apertured dielectric probe (aluminum or gold coated multimode pulled fiber) of a near field scanning optical microscope (NSOM) [3], the semiconductor (typically silicon nitrite) microcantilever of an atomic force microscope (AFM) [4], or the dielectric probe (a multimode pulled fiber) of a photon scanning tunneling microscope (PSTM) [5], and the metallic probe (atomically sharp tungsten) of a scanning tunneling microscope (STM) [6] may all be candidate problems for the investigation presented here. For further discussions on how these systems may be modeled in the geometry discussed in this manuscript see references [7]-[9].

Furthermore, in many manufactured nanoparticles such as carbon nanohorn, nanotubes, metal dimers, metal-insulator-metal tunnel junctions, noble metal nanorings, etc., electron confinement in surfaces or bulk of $\mathbf{O}_i, i \in \mathbb{N}$ results in surface modes [2] that can be obtained by solving the appropriate boundary value problem such as Schrödinger's or Laplace's equations in spheroidal, hyperboloidal, and toroidal spaces. In such instances, the monotonic radial functions $w(r)$ associated with the solutions to, for example, Laplace's equation in spherical coordinates appropriate for satisfaction of boundary conditions at fixed radial values become oscillatory when a boundary condition has to be satisfied at some initial r_i and final r_f value, that is, in an interval $r \in [r_i, r_f]$. This is tied to the complex eigenvalues of the problem associated with particular choice of the separation constant. Likewise, oscillatory angular eigenfunctions become monotonic when satisfaction of the boundary condition restricts the value of the angular coordinate to a fixed value. In particular, the discrete eigenvalues of a system become continuous when one dimension of the system becomes infinite. Such behavior of eigenvalues is of importance for a particular type of surface excitation, which is due to the quantum mechanical effect of collective electronic oscillations in certain metals. The quanta of these oscillations are called surface plasmons. In the geometries considered here, the fractional index of the kernel of the index transforms, can be shown to be closely related to the momentum of a plasmon.

The goal of this manuscript is to disseminate the usefulness of index transforms in modeling of nanostructures so as to somewhat bridge the gap between the current experiments and the theoretical modeling. We have chosen SPM as the experimental platform due to the fact that the shape of many SPM probes can be approximated with a hyperboloid. The Cartesian cases are mentioned due to the ability of a special confocal hyperboloid to become a plane, see Fig. 6, Fig. 7, and Fig. 8 .

In order to elucidate the application of the index transform and their kernel conical functions in the modeling of problems involving $\mathbf{O}_i, i \in \mathbb{N}$, we have organized our presentation as follows. In section II we study the Laplace equation for a hyperboloid, and in section III, for a conical case. Appendices A and B provide useful relations used throughout the manuscript and a conclusion is given in section IV. In doing so, we first describe the hyperboloidal geometry in subsection II A, and set up the Laplacian and obtain a general solution to Laplace equation in subsection II B. The nature of the separation variable used in subsection II B requires special attention and subsection II C has been devoted to this topic. We then proceed by setting up a boundary value problem in subsection II D and define and use the Mehler-Fock transform, to obtain a formal solution (pertaining to the case depicted in Fig. 3-left) in subsection II E, where we also provide a specific example of an

experimentally relevant boundary condition that can be handled using the results. Section II ends with subsection II F, where a rigorous treatment of the Mehler-Fock transform of arbitrary order m is presented and the previous example of a specific boundary condition is revisited. We then briefly discuss the conical case in Section III for the sake of comparison and further properties of the conical functions. We end section III with yet another example of an experimentally useful potential distribution on a conical probe.

II. HARMONIC FUNCTIONS IN HYPERBOLOIDAL DOMAINS AND PROLATE SPHEROIDAL SYSTEM

We begin by displaying a scanning electron microscope (SEM) image of an optical (SPM) probe and the corresponding modeling geometry in Fig. 3. Stating that further discussions may be found in the work of Lebedev[10], Yakubovich[11], Zayed[12], Sneddon[13], Morse and Feshbach[14], Virchenko and Fedotova[15], and Mandal[16], we proceed by defining the degenerate ellipsoidal coordinates or the spheroidal coordinates in which one set of coordinates is a set of confocal two-sheeted hyperboloids of revolution (prolate spheroidal coordinates). The orthogonal surfaces are confocal prolate spheroids, see Fig. 6.

A. The Geometry

Consider the orthogonal coordinate system (ζ, θ, φ), shown in Fig. 6 and Fig. 7, and defined via the following connection to the Cartesian coordinates:

$$\begin{aligned} x(\zeta,\theta,\varphi) &= z_0 \sinh\zeta \sin\theta \cos\varphi, \\ y(\zeta,\theta,\varphi) &= z_0 \sinh\zeta \sin\theta \sin\varphi, \\ z(\zeta,\theta,\varphi) &= z_0 \cosh\zeta \cos\theta, \end{aligned} \tag{1}$$

with ζ, θ, and φ running in the intervals:

$$0 \le \zeta < \infty, \qquad 0 \le \theta \le \pi, \qquad 0 \le \phi < 2\pi, \tag{2}$$

and $z_0 > 0$ is a scale factor with a metric unit, which explicitly sets the metric units for the distance between two arbitrary points in space. As is evident from equation (1), the effect of a variation in z_0 corresponds to zooming in or out over an arbitrary region of space. For convenience we set:

$$\begin{aligned} \cosh\zeta &= \eta, \quad 1 \le \eta < \infty, \\ \cos\theta &= \mu, \quad -1 \le \mu \le 1, \end{aligned} \tag{3}$$

which rewrites (1) as:

$$\begin{aligned} x(\eta,\mu,\varphi) &= z_0 \sqrt{(\eta^2-1)(1-\mu^2)} \cos\varphi, \\ y(\eta,\mu,\varphi) &= z_0 \sqrt{(\eta^2-1)(1-\mu^2)} \sin\varphi, \\ z(\eta,\mu,\varphi) &= z_0 \eta\mu. \end{aligned} \tag{4}$$

In terms of cylindrical coordinates (ρ, φ, z) with:

$$(x, y, z) = (\rho\cos\varphi, \rho\sin\varphi, z),$$

the transformation in (1) can be expressed as:

$$z + i\rho = z_0 \cosh(\zeta + i\theta). \tag{5}$$

Further information is provided in the appendix.

The utility of the description above can be captured in the modeling of a complex SPM probe-substrate ($\mathbf{O_1}$-$\mathbf{O_2}$) system shown in Fig. 8. When solving, for example Laplace's equation, index transform facilitates the satisfaction of the boundary conditions on the surfaces of $\mathbf{O_1}$ and $\mathbf{O_2}$ in Fig. 8.

B. Laplacian and Separation of Variables

Using (A13), Laplace's equation $\Delta\Phi(\bar{r}) = 0$ takes the form:

$$\frac{\partial}{\partial\eta}\left[(\eta^2-1)\frac{\partial\Phi}{\partial\eta}\right] + \frac{\partial}{\partial\mu}\left[(1-\mu^2)\frac{\partial\Phi}{\partial\mu}\right] + \left[\frac{1}{1-\mu^2} + \frac{1}{\eta^2-1}\right]\frac{\partial^2\Phi}{\partial\varphi^2} = 0, \tag{6}$$

which is separated with the ansatz:

$$\Phi(\bar{r}) = \Phi(\eta,\mu,\varphi) = f(\eta)g(\mu)h(\varphi). \tag{7}$$

The azimuthal part of Laplace's equation can now be easily separated. A separation constant m is used, which is restricted to integer values in order for $g(\varphi)$ to be single valued and oscillatory, that is:

$$\frac{d^2h(\varphi)}{d\varphi^2} + m^2h(\phi) = 0 \Rightarrow h(\varphi) \propto e^{\pm imp}, \quad \varphi \in [0, 2\pi],\ m = 0, 1, 2, \cdots. \tag{8}$$

Thus the general solution can be expanded as a Fourier series in the azimuthal variable φ as [13], [17]:

$$\Phi(\eta,\mu,\phi) = \sum_0^\infty f_m(\eta)g_m(\mu)(2-\delta_m^0)\cos m\phi. \tag{9}$$

Introducing the second separation constant c, f_m and g_m will satisfy the following partial differential equation:

$$\begin{aligned} \frac{d}{d\eta}\left[(\eta^2-1)\frac{df_m(\eta)}{d\eta}\right] - \frac{m^2}{\eta^2-1}f_m(\eta) &= cf_m(\eta), \\ \frac{d}{d\mu}\left[(1-\mu^2)\frac{dg_m(\mu)}{d\mu}\right] - \frac{m^2}{1-\mu^2}g_m(\mu) &= -cg_m(\eta). \end{aligned} \tag{10}$$

The possibility of obtaining a continuous spectrum of real eigenvalues and eigenfunctions relies on setting $c = \nu(\nu+1)$, (this particular selection is a consequence of the necessary criteria for existence of the eigenvalues and is discussed in [18] and [19]) with ν given by the following complex number (see next section):

$$\nu = -\frac{1}{2} + iq \Rightarrow c = -\frac{1}{4} - q^2, \tag{11}$$

where q is a continuous variable $q \in [0, \infty[$, appropriate for the infinite surface of a hyperboloid as opposed to the discrete values of ν arising in the case of bounded surfaces. The ODEs in (10) are now written, using (11), as:

$$\begin{aligned} &\frac{d}{d\eta}\left[(\eta^2-1)\frac{df_m(\eta)}{d\eta}\right] - \left[\frac{m^2}{\eta^2-1} - \left(q^2+\frac{1}{4}\right)\right] f_m(\eta) = 0, \\ &\frac{d}{d\mu}\left[(1-\mu^2)\frac{dg_m(\mu)}{d\mu}\right] - \left[\frac{m^2}{1-\mu^2} + \left(q^2+\frac{1}{4}\right)\right] g_m(\mu) = 0, \end{aligned} \tag{12}$$

which are solved by the conical functions $P^m_{-\frac{1}{2}+iq}(z)$, also called as associated Legendre functions with continuous complex lower index (see Appendix for more details). The argument $z \in]-\infty, \infty[$ is set to $z = \eta = \cosh\zeta$ to give the solution to the first equation in (12) while it takes on $z = \pm\mu = \pm\cos(\theta)$ to generate the two linearly independent solutions of the second equation in (12). Using the recursion relations for the conical functions, it can be shown that the differential equations in (12) are satisfied by the conical functions.

Thus, the general solution is written as the following infinite series over the infinite integrals:

$$\begin{aligned} \Phi(\bar{r}) = &\sum_{m=0}^{\infty} h_m(\varphi) \\ &\times \int_0^{\infty} P^m_{-\frac{1}{2}+iq}(\cosh\zeta)\left[A_m(q)P^m_{-\frac{1}{2}+iq}(\cos\theta) + B_m(q)P^m_{-\frac{1}{2}+iq}(-\cos\theta)\right] dq, \end{aligned} \tag{13}$$

where the azimuthal functions $h_m(\varphi)$ are given by

$$h_m(\varphi) = (2-\delta^m_0)\,\cos m\varphi. \tag{14}$$

C. The Form of ν

Following Lebedev [20], we first show why the separation variable has to take the particular form of $-1/2 + iq$ and briefly discuss the nature of these eigenvalues and their behavior and physical interpretation. Our proof here is similar to the one discussed by Belova and Ufliand [19], and N. I. Sneddon [13]. As derived above, see (6), in order to solve the Laplace equation in toroidal coordinates (α, η, φ) or spheroidal coordinates (ζ, θ, φ), using the separation of variables, one has to deal with the singular boundary value problem:

$$(1-z^2)\frac{d^2u}{dz^2} - 2z\frac{du}{dz} + \left[\nu(\nu+1) - \frac{\mu^2}{1-z^2}\right] u = 0 \tag{15}$$

subject to the conditions

$$\begin{cases} 1 \le z_0 < z < \infty \\ u(z_0) = 0 \\ u(\infty) = 0, \end{cases} \tag{16}$$

where $z = \cosh\alpha$ in toroidal coordinates or $z = \cosh\zeta$ in spheroidal coordinates and μ denotes one of the discrete real eigenvalues obtained from the solutions of boundary value problem in the variable φ common to both coordinate systems, which can be assumed to be non–negative. Note also that in this section we do not assume μ to be necessarily a non–negative integer.

We start by showing that there are no eigenvalues for the boundary value problem (15) and (16) in the right half–plane Re $\nu > 0$. It is known that the associated Legendre functions of first and second kind denoted by $P_\nu^\mu(z)$ and $Q_\nu^\mu(z)$ are the two linearly independent solutions of (15). The asymptotic behaviors of $P_\nu^\mu(z)$ and $Q_\nu^\mu(z)$ for large values of z (see [21], formula 8.776) implies that $Q_\nu^\mu(z)$ is the only eigenfunction satisfying the last condition in (16). Therefore, the eigenvlues are given by $Q_\nu^\mu(z_0) = 0$. However, $Q_\nu^\mu(z)$ has no real zeros exceeding 1 for $\nu > -\frac{3}{2}$ and $\nu + \mu + 1 > 0$ (see for example [21], formula 8.783). Thus, the eigenvalues in the right half–plane Re $\nu > 0$, if any, must be complex. Assuming ν and $\bar{\nu}$ are a pair of conjugate complex eigenvlues, twice integration of equation (15) together with the boundary condition $Q_\nu^\mu(z_0) = 0$ implies

$$(\lambda - \bar{\lambda}) \lim_{z\to\infty} \int_{z_0}^{z} |Q_\nu^\mu(z)|^2 \, dz = \lim_{z\to\infty} (z^2 - 1) \left[Q_\nu^\mu(z) \overline{Q_\nu^\mu(z)}' - \overline{Q_\nu^\mu(z)} Q_\nu^\mu(z)' \right], \tag{17}$$

where $\lambda = \nu(\nu + 1)$. Using the fact (see for example Gradshteyn and Ryzhik 8.732)

$$(z^2 - 1) \frac{dQ_\nu^\mu(z)}{dz} = (\nu - \mu + 1) Q_{\nu+1}^\mu(z) - (\nu + 1) z Q_\nu^\mu(z),$$

and the asymptotic behavior of $Q_\nu^\mu(z)$ for $z \gg 1$, we have that the magnitude of the last expression in (17) is of order $z^{-2\nu-3}$ for large values of z. As result, the right hand side of (17) should vanish for any fixed ν with non–negative real part. But this would imply $Q_\nu^\mu(z) = 0$, a contradiction.

Clearly the equation (15) will remain the same if one substitutes ν by $-\nu - 1$. Therefore, we have the same eigenvlues for both ν and $-\nu - 1$. But we have just proved that the boundary value problem (15) and (16) has no eigenvalue in the right half–plane. Thus for any eigenvalue ν we must have that Re $\nu \leq 0$ and Re $\{-\nu - 1\} \leq 0$, which is only satisfied in the strip

$$-1 < \text{Re } \nu \leq 0.$$

(Note the strict inequality since $\nu = 0$ and $\nu = -1$ give rise to the same eigenvalue.)

In the strip $-1 < \text{Re } \nu \leq 0$, the eigenfunction to the boundary value problem (15) and (16) is a linear combination of $P_\nu^\mu(z)$ and $Q_\nu^\mu(z)$ with continuous spectrum of eigenvalues. Finally if we let $\nu = -\frac{1}{2} + iq$, then we have real–valued eigenvalues $\nu(\nu + 1) = q^2 - \frac{1}{4}$ and real–valued eigenfunctions $P^\mu_{-\frac{1}{2}+iq}(z)$ and $Q^\mu_{-\frac{1}{2}+iq}(z)$.

D. The Boundary Value Problem

It is straightforward to show from Maxwell's equation that, without any source terms, in the time-independent limit (speed of light $c \to \infty$), the distribution of the scalar potential Φ of the electric field in domains containing a probe and a sample/substrate (such as those depicted in figures 1-8) is given by the solution to

$$\begin{cases} \nabla \cdot \epsilon \nabla \Phi(\mathbf{r}) = 0 & : \quad \Omega, \\ \Phi(\mathbf{r}) = f(\mathbf{r}) & : \quad \partial\Omega, \end{cases} \tag{18}$$

where, ϵ is the dielectric function characterizing the medium in the subdomains Ω such that

$$\begin{cases} \Omega_I & : \quad \theta < \theta_t < \frac{\pi}{2} \quad : \quad \mathbf{O_1}(\text{probe}), \\ \Omega_{II} & : \quad \theta > \frac{\pi}{2} \quad : \quad \mathbf{O_2}(\text{substrate}). \end{cases} \tag{19}$$

The boundary $\partial\Omega = \partial\Omega_I \cup \partial\Omega_{II}$ is given by

$$\begin{cases} \partial\Omega_I & : \quad \theta = \theta_t \quad \text{(probe boundary)}, \\ \partial\Omega_{II} & : \quad \theta = \frac{\pi}{2} \quad \text{(substrate surface)}, \end{cases} \tag{20}$$

where θ_t is a fixed value of the angular variable θ and $f(\mathbf{r})$ is a prescribed function in close resemblance with an experimentally imposed quasi-static potential. With fixed values $\theta = \theta_t$ and $\theta = \pi/2$, equation (19) map the tip hyperboloid and the xy–plane, respectively (see for example Fig. 3-left or the more elaborate system in Fig. 8).

In the present case we are specifically interested in the following boundary conditions:

$$\begin{cases} \Phi(\mathbf{r}) = f(\mathbf{r}) & : \partial\Omega_I \\ \hat{z} \cdot \epsilon\nabla\Phi(\mathbf{r}) = 0, \quad \mathbf{R} \cdot \nabla\Phi(\mathbf{r}) = 0 & : \partial\Omega_{II} \end{cases} \tag{21}$$

where $\mathbf{R} = (x, y, 0)$. Nevertheless, our result is easily adopted to a more general problem with the following boundary conditions:

$$\begin{cases} \Phi(\mathbf{r}) = f(\mathbf{r}) & : \partial\Omega_I \\ \hat{n} \cdot \epsilon\nabla\Phi(\mathbf{r}) = 0, \quad \hat{t} \cdot \nabla\Phi(\mathbf{r}) = 0 & : \partial\Omega_{II} \end{cases} \tag{22}$$

where $\hat{n}(\hat{t})$ is a normal (tangential) unit vector to the probe's surface, important for the case of an isolated probe interacting with a charged substrate. For example, f can then represent the potential of a surface dipole.

E. Solution of the Boundary Value Problem and the Mehler-Fock transform

Using (13) and the properties of the conical functions $P^m_{-\frac{1}{2}+iq}(\cos\theta)$ one can write the general solution to the boundary value problem (18)–(20) as

$$\Phi(\mathbf{r}) = \sum_{m=0}^{\infty} h_m(\varphi) \int_0^{\infty} P^m_{-\frac{1}{2}+iq}(\cosh\zeta) u^m_q(\cos\theta)\, dq, \tag{23}$$

where $h_m(\varphi)$ is as before and

$$u^m_q(\cos\theta) = \begin{cases} C^m_q P^m_{-\frac{1}{2}+iq}(\cos\theta) + D^m_q P^m_{-\frac{1}{2}+iq}(-\cos\theta) & : \Omega_I \\ E^m_q P^m_{-\frac{1}{2}+iq}(-\cos\theta) & : \Omega_{II} \end{cases} \tag{24}$$

Taking the $z = 0$ plane as the boundary of a hyperboloid with an angle $\pi/2$ (or a cone with half angle $\pi/2$), the second condition; that is, the continuity of the normal component of the displacement field $\mathbf{D} = \epsilon\nabla\Phi(\mathbf{r})$ due to lack of free charges at $\partial\Omega_{II}$, and the continuity of the tangential component of the electric field $\mathbf{E} = \nabla\Phi(\mathbf{r})$; or equivalently, the continuity of the scaler potential $\Phi(\mathbf{r})$, results in

$$0 = \sum_{m=0}^{\infty} h_m(\varphi) \int_0^{\infty} dq P^m_{-\frac{1}{2}+iq}(\cosh\zeta) \times \begin{cases} \Lambda \\ \Lambda' \end{cases}, \tag{25}$$

where

$$\Lambda = (C^m_q + D^m_q - E^m_q)\, P^m_{-\frac{1}{2}+iq}(0), \tag{26}$$

$$\Lambda' = (\epsilon_I C^m_q - \epsilon_I D^m_q + \epsilon_{II} E^m_q)\, \left.\frac{\partial P^m_{-\frac{1}{2}+iq}(\cos\theta)}{\partial\cos\theta}\right|_{\theta=\pi/2}.$$

In writing the second equation, we have utilized the generating function of the conical function (B7). Thus, $\forall r \in [0, \infty)$, the orthogonality of the azimuthal and the conical functions yields $\Lambda = \Lambda' = 0$, and we write

$$u_q^m(\cos\theta) = D_q^m \, v_q^m(\cos\theta), \tag{27}$$

where

$$v_q^m(\cos\theta) = \begin{cases} \alpha(\epsilon) P^m_{-\frac{1}{2}+iq}(\cos\theta) + P^m_{-\frac{1}{2}+iq}(-\cos\theta) & : \Omega_I \\ \beta(\epsilon) P^m_{-\frac{1}{2}+iq}(-\cos\theta) & : \Omega_{II} \end{cases} \tag{28}$$

and

$$\alpha(\epsilon) = \frac{\epsilon_I - \epsilon_{II}}{\epsilon_I + \epsilon_{II}}, \quad \beta(\epsilon) = \frac{2\epsilon_I}{\epsilon_I + \epsilon_{II}}. \tag{29}$$

Now, the satisfaction of the boundary condition at the probe; that is, condition (21) or (22) on $\partial\Omega_I$, implies $f(\zeta, \varphi) = \Phi(\zeta, \theta_t, \varphi)$. Therefore, using (23) and (27) for the probe boundary $\partial\Omega_I$, we must have

$$f(\zeta, \varphi) = \sum_{m=0}^{\infty} h_m(\varphi) \int_0^{\infty} D_q^m \, v_q^m(\cos\theta_t) \, P^m_{-\frac{1}{2}+iq}(\cosh\zeta) \, dq, \tag{30}$$

where

$$v_q^m(\cos\theta_t) = v_q^m(\cos\theta)\big|_{\partial\Omega_I} = \alpha(\epsilon) P^m_{-\frac{1}{2}+iq}(\cos\theta_t) + P^m_{-\frac{1}{2}+iq}(-\cos\theta_t). \tag{31}$$

Assuming that for each fixed $\zeta > 0$, f is φ–integrable on the interval $[0, 2\pi]$, it follows from the classical result on Fourier series that

$$f_m(\zeta) = \frac{1}{2\pi} \int_0^{2\pi} f(\zeta, \varphi) h_m(\varphi) \, d\varphi = \int_0^{\infty} D_q^m \, v_q^m(\cos\theta_t) \, P^m_{-\frac{1}{2}+iq}(\cosh\zeta) \, dq. \tag{32}$$

It is also worth mentioning that for each fixed $\zeta > 0$, equality (30) holds at every continuity point of f with respect to φ, and the right side of (30) converges to the average of f with respect to φ at the point of discontinuity. Moreover at those ζ where f is continuous with respect to φ on $[0, 2\pi]$, the series in (30) converges uniformly and absolutely (see any classical reference on this topic).

Finally, the calculation of D_q^m is facilitated by the use of the Mehler–Fock index transform of the order $m \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$ (see [13] and/or [11]) defined by

$$\mathcal{J}_m(q) = \int_1^{\infty} f(\eta) P^{-m}_{-\frac{1}{2}+iq}(\eta) d\eta, \tag{33}$$

with the inverse transformation (see [12] pp. 415–426)

$$f(\eta) = (-1)^m \int_0^{\infty} q \tanh(\pi q) \mathcal{J}_m(q) P^m_{-\frac{1}{2}+iq}(\eta) \, dq, \tag{34}$$

where $q \geq 0$ and

$$P^{-m}_{-\frac{1}{2}+iq}(\cosh\xi) = \sqrt{\frac{2}{\pi}} \frac{\sinh^{-m}\xi}{\Gamma(1/2+m)} \int_0^{\xi} \frac{\cos\alpha q}{(\cosh\xi - \cosh\alpha)^{1/2-m}} d\alpha \quad (\xi > 0) \tag{35}$$

denotes the usual associated Legendre or conical function (see [15]). If $m = 0$, we simply denote $P^{\,0}_{-\frac{1}{2}+iq}(\eta)$ by $P_{-\frac{1}{2}+iq}(\eta)$.

In the next section, we will fully discuss the conditions under which the Mehler–Fock transform of order m exists and give necessary conditions for the inverse formula to hold. In this section, however, we make the assumption that the inverse formula (34) holds for each $f_m(\zeta)$ in (32). It follows now from (32), (33), and (34) that

$$D_q^m = \frac{(-1)^m q \tanh(\pi q)}{v_q^m(\cos\theta_t)} \int_0^\infty f_m(\zeta) P^{-m}_{-\frac{1}{2}+iq}(\cosh\zeta) \sinh\zeta \, d\zeta. \tag{36}$$

Thus the solution to the boundary value problem (18)–(20) is given by

$$\Phi(\mathbf{r}) = \sum_{m=0}^{\infty} (-1)^m h_m(\varphi) \int_0^\infty \frac{v_q^m(\cos\theta)}{v_q^m(\cos\theta_t)} \, q \tanh(\pi q) \, F_m(q) P^m_{-\frac{1}{2}+iq}(\cosh\zeta) \, dq, \tag{37}$$

where $h_m(\varphi)$ and $v_q^m(\cos\theta)$ are given by (14) and (28), respectively, and

$$F_m(q) = \int_0^\infty f_m(\zeta) P^{-m}_{-\frac{1}{2}+iq}(\cosh\zeta) \sinh\zeta \, d\zeta \tag{38}$$

where

$$f_m(\zeta) = \frac{1}{2\pi} \int_0^{2\pi} f(\zeta, \varphi) h_m(\varphi) \, d\varphi. \tag{39}$$

We now proceed by studying a specific example, where the boundary function f is axially symmetric, that is, $f(\zeta, \varphi) = f(\zeta)$. As a result, the solution reduces to the case $m = 0$ and calculation of

$$F(q) = F_0(q) = \int_0^\infty f(\zeta) P_{-\frac{1}{2}+iq}(\cosh\zeta) \sinh\zeta \, d\zeta, \tag{40}$$

or equivalently

$$F(q) = \int_1^\infty f(\eta) P_{-\frac{1}{2}+iq}(\eta) \, d\eta. \tag{41}$$

As an example, assuming V_0 to be a constant potential (corresponding to a charged probe), and γ to be a constant spatial decay rate, we examine the function

$$f(\eta) = V_0 e^{-\gamma\eta}, \tag{42}$$

which has the Mehler–Fock integral transform (see for example (7-6-22) in [13] or (2.17.7.1) in [22])

$$\sqrt{\frac{2}{\pi\gamma}} \, K_{iq}(\gamma) = \int_1^\infty e^{-\gamma\eta} P_{-\frac{1}{2}+iq}(\eta) \, d\eta, \tag{43}$$

where $K_{iq}(\gamma)$ are the MacDonald's function, which can be expressed in terms of their Fourier cosine transform

$$K_{iq}(\gamma) = \int_0^\infty e^{-\gamma\cosh\zeta} \cos(q\zeta) \, d\zeta. \tag{44}$$

Thus, using (37), we can write the solution as

$$\Phi(\mathbf{r}) = \sqrt{\frac{2}{\pi\gamma}} \int_0^\infty \frac{v_q^0(\cos\theta)}{v_q^0(\cos\theta_t)} \, q \tanh(\pi q) \, K_{iq}(\gamma) P_{-\frac{1}{2}+iq}(\cosh\zeta) \, dq. \tag{45}$$

F. Existence and Inversion Theorems for the Mehler-Fock Transform of Order $m \in \mathbb{N}_0$

In what follows, we give a formal operational proof motivated by Sneddon (see [13], pp. 415-416) to provide natural sufficient conditions on a class of functions f, where the inversion formula or a unique solution of the integral equation (33) holds. As a consequence, we give an answer to Sneddon's question regarding the absence of such conditions for the Mehler–Fock transformation of general order $m \in \mathbb{N}_0$. Note that the classical case $m = 0$ was investigated in details by Lebedev [23] and [10]. Further results with conditions on $\mathcal{J}_m(q)$ can also be found in the works of Olevskii [24] and Vilenkin [25]. The L_2, L_p–versions of this transformation were studied in [26], [11], [27], and [28].

1. Sneddon's Operational Method

We state our existence theorems in two parts based on the extra conditions needed for cases m=0, 1, and 2. Recall that $C_0(0,\infty)$ denotes the space of continuous functions vanishing at infinity and $C_0^{(k)}(0,\infty)$, $k \geq 1$, stand for the spaces of k–times continuously differentiable functions vanishing at infinity.

Theorem 1 (Existence Theorem part I)**.** *Let f be a locally integrable function on $(1,\infty)$; i.e. $f \in L_1^{loc}(1,\infty)$, satisfying the asymptotic conditions*

$$f(\eta) = \begin{cases} O((\eta-1)^a) & \text{as } \eta \to 1+, \\ O(\eta^b) & \text{as } \eta \to \infty, \end{cases} \tag{46}$$

where

$$a + \frac{m}{2} > -1 \quad \text{and} \quad b + \frac{1}{2} < 0 \quad (m \in \mathbb{N}_0). \tag{47}$$

Then the Mehler–Fock transform $\mathcal{J}_m(q)$ is well–defined as an absolutely and uniformly convergent integral for all $m \in \mathbb{N}_0$. Moreover, for each fixed $m \geq 0$, $\mathcal{J}_m(q)$ belongs to $C_0^{(k)}(0,\infty)$ for all $k \geq 0$. If $m \geq 3$, then $\mathcal{J}_m(q)$ has the asymptotic behavior

$$\mathcal{J}_m(q) = O\left(\frac{1}{q^3}\right) \quad \text{as} \quad q \to \infty. \tag{48}$$

Proof. Throughout the proof, note that we will switch between the two variables η and ξ related by the equality $\eta = \cosh\xi$. Fix $m \in \mathbb{N}_0$. Substituting (35) in (33) and using Fubini's Theorem for non-negative integrands imply that

$$\begin{aligned} |\mathcal{J}_m(q)| &\leq \sqrt{\frac{2}{\pi}} \frac{1}{\Gamma(1/2+m)} \int_0^\infty \int_\alpha^\infty \frac{|f(\cosh\xi)| \sinh^{1-m}\xi}{(\cosh\xi - \cosh\alpha)^{1/2-m}} d\xi \, d\alpha \\ &= \sqrt{\frac{2}{\pi}} \frac{1}{\Gamma(1/2+m)} \int_0^\infty |f(\cosh\xi)| \sinh^{1-m}\xi \int_0^\xi \frac{d\alpha}{(\cosh\xi - \cosh\alpha)^{1/2-m}} d\xi \\ &\leq \frac{\sqrt{\pi}}{\Gamma(1/2+m)} \int_1^\infty |f(\eta)| (\eta^2-1)^{-m/2} (\eta-1)^m P_{-\frac{1}{2}}(\eta) d\eta. \end{aligned} \tag{49}$$

Now, taking into account that (see [21] 8.7–8.8)

$$P_{-\frac{1}{2}}(\eta) = O(1) \text{ as } \eta \to 1+ \quad \text{and} \quad P_{-\frac{1}{2}}(\eta) = \eta^{-1/2} \text{ as } \eta \to \infty,$$

it follows from our assumptions (46) and (47) that the last expression in (49) is finite. This proves that $\mathcal{J}_m(q)$ belongs to $C_0(0,\infty)$. For any fixed $k \geq 0$, a similar argument as in (49) shows that

$$\begin{aligned}\left|\mathcal{J}_m^{(k)}(q)\right| &\leq \sqrt{\frac{2}{\pi}}\frac{1}{\Gamma(1/2+m)}\int_0^\infty \alpha^k \int_\alpha^\infty \frac{|f(\cosh\xi)|\sinh^{1-m}\xi}{(\cosh\xi-\cosh\alpha)^{1/2-m}}d\xi\ d\alpha \\ &= \sqrt{\frac{2}{\pi}}\frac{1}{\Gamma(1/2+m)}\int_0^\infty |f(\cosh\xi)|\sinh^{1-m}\xi \int_0^\xi \frac{\alpha^k d\alpha}{(\cosh\xi-\cosh\alpha)^{1/2-m}}d\xi \\ &\leq \frac{\sqrt{\pi}}{\Gamma(1/2+m)}\int_1^\infty |f(\eta)|(\eta^2-1)^{-m/2}(\eta-1)^m P_{-\frac{1}{2}}(\eta)\ \log^k\left(\eta+\sqrt{\eta^2-1}\right)d\eta < \infty,\end{aligned}$$

where the last estimate holds under the extra assumption $a+\frac{k+m}{2} > -1$. But this trivially follows from (47). Therefore we have $\mathcal{J}_m(q) \in C_0^{(k)}(0,\infty)$.

Here, we observe that (49) implies one can reverse the order of integration in the definition of (33) and rewrite $\mathcal{J}_m(q)$ as

$$\mathcal{J}_m(q) = \sqrt{\frac{2}{\pi}}\frac{1}{\Gamma(1/2+m)}\int_0^\infty \cos\alpha q \int_\alpha^\infty \frac{f(\cosh\xi)\sinh^{1-m}\xi}{(\cosh\xi-\cosh\alpha)^{1/2-m}}\,d\xi\,d\alpha. \tag{50}$$

Now the proof of (48) can be accomplished by three successive applications of integration by parts starting with the equality (50). Let

$$dF(\alpha) = \cos\alpha q\,d\alpha$$

and

$$G(\alpha) = \int_\alpha^\infty \frac{f(\cosh\xi)\sinh^{1-m}\xi}{(\cosh\xi-\cosh\alpha)^{1/2-m}}\,d\xi.$$

Clearly F vanishes at zero. Moreover, using assumption (46) on the asymptotic behavior of f for large η, it follows from the estimate

$$\begin{aligned}\left|\int_\alpha^\infty \frac{f(\cosh\xi)\sinh^{1-m}\xi}{(\cosh\xi-\cosh\alpha)^{1/2-m}}d\xi\right| &\leq \int_\alpha^\infty |f(\eta)|(\eta^2-1)^{-m/2}(\eta-1)^{m-1/2}d\eta \\ &= O\left(\int_\alpha^\infty \eta^{b-1/2}d\eta\right),\end{aligned}$$

and $b+\frac{1}{2} < 0$ that G also vanishes at infinity. Therefore the integration by parts in (50) with respect to α yields

$$\mathcal{J}_m(q) = \sqrt{\frac{2}{\pi}}\frac{q^{-1}}{\Gamma(m-1/2)}\int_0^\infty \sinh\alpha\sin\alpha q\int_\alpha^\infty \frac{f(\cosh\xi)\sinh^{1-m}\xi}{(\cosh\xi-\cosh\alpha)^{3/2-m}}d\xi\ d\alpha. \tag{51}$$

The latter iterated integral is absolutely and uniformly convergent due to the estimate

$$\begin{aligned}&\int_0^\infty \sinh\alpha\int_\alpha^\infty \frac{|f(\cosh\xi)|\sinh^{1-m}\xi}{(\cosh\xi-\cosh\alpha)^{3/2-m}}\,d\xi\,d\alpha \\ &\qquad= \int_0^\infty |f(\cosh\xi)|\sinh^{1-m}\xi\int_0^\xi \frac{\sinh\alpha}{(\cosh\xi-\cosh\alpha)^{3/2-m}}d\alpha\,d\xi \\ &\qquad\leq \frac{\pi}{\sqrt{2}}\int_0^\infty |f(\cosh\xi)|\sinh^{2-m}\xi\ (\cosh\xi-1)^{m-1}P_{-\frac{1}{2}}(\cosh\xi)\,d\xi \\ &\qquad= \int_1^\infty |f(\eta)|(\eta-1)^{(m-1)/2}\ (\eta+1)^{(1-m)/2}P_{-\frac{1}{2}}(\eta)d\eta < \infty,\end{aligned}$$

where in the last estimate we have used assumptions (46) and (47). Another integration by parts with respect to α in (51), where

$$dF(\alpha) = \cos \alpha q \, d\alpha$$

and

$$G(\alpha) = \sinh \alpha \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{3/2-m}} \, d\xi,$$

together with the estimate

$$\begin{aligned} \sinh \alpha \left| \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{3/2-m}} d\xi \right| &\leq \frac{\sinh \alpha}{\cosh \alpha - 1} \int_\alpha^\infty |f(\eta)| (\eta^2 - 1)^{-m/2} (\eta - 1)^{m-1/2} d\eta \\ &= O\left(\int_\alpha^\infty \eta^{b-1/2} d\eta \right) \to 0 \qquad \alpha \to \infty, \end{aligned}$$

where $b + \frac{1}{2} < 0$, gives

$$\begin{aligned} \mathcal{J}_m(q) = \sqrt{\frac{2}{\pi}} \frac{q^{-2}}{\Gamma(m - 1/2)} \int_0^\infty \cosh \alpha \cos \alpha q \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{3/2-m}} d\xi \; d\alpha \\ - \sqrt{\frac{2}{\pi}} \frac{q^{-2}}{\Gamma(m - 3/2)} \int_0^\infty \sinh^2 \alpha \cos \alpha q \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{5/2-m}} d\xi \; d\alpha. \end{aligned} \tag{52}$$

Using a similar argument as the one given for (51) one can show that the iterated integrals in (52) are convergent absolutely and uniformly under the assumptions (46) and (47) of the theorem. Finally, we use integration by parts in (52). Since the elimination of the free terms uses the same techniques already explained in (51) and (52), we omit their proofs here. Thus we get

$$\begin{aligned} \mathcal{J}_m(q) = &- \sqrt{\frac{2}{\pi}} \frac{q^{-3}}{\Gamma(m - 1/2)} \int_0^\infty \sinh \alpha \sin \alpha q \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{3/2-m}} \, d\xi \, d\alpha \\ &+ \frac{3}{\sqrt{2\pi}} \frac{q^{-3}}{\Gamma(m - 3/2)} \int_0^\infty \sinh 2\alpha \sin \alpha q \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{5/2-m}} \, d\xi \, d\alpha \\ &- \sqrt{\frac{2}{\pi}} \frac{q^{-3}}{\Gamma(m - 5/2)} \int_0^\infty \sinh^3 \alpha \sin \alpha q \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{7/2-m}} \, d\xi \, d\alpha, \end{aligned} \tag{53}$$

under conditions (46) and (47) of the theorem. This completes the proof of (48). □

In general, it is impossible to differentiate under the integral sign as we did in (51), (52), and (53). Therefore, we must use a different argument in order to prove (48) for the cases $m = 0, 1, 2$. Now let us consider again the equality (50). The same argument regarding the integration by parts in (51) implies

$$\mathcal{J}_m(q) = - \sqrt{\frac{2}{\pi}} \frac{1}{q \Gamma(1/2 + m)} \int_0^\infty \sin \alpha q \frac{d}{d\alpha} \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{1/2-m}} d\xi \; d\alpha, \tag{54}$$

where in the above equality we have not differentiated under the integral sign. However, for $m \neq 0$, the latter equality (54) can be written in the form (51). Next, we denote by

$$\varphi_m(\alpha) = \sqrt{\frac{2}{\pi}} \frac{1}{\Gamma(1/2 + m)} \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{1/2-m}} \, d\xi, \tag{55}$$

the inner integral in (54). In fact, $\varphi_m(\alpha)$ is called a fractional integral operator of an integrable function $f(\cosh\xi)\sinh^{-m}\xi$ by function $\cosh\alpha$ on the half–axis [29]. Before stating the second part of our Existence Theorem, we need one more definition.

Definition. A function φ is said to belong to the class $AC^3(0,\infty)$ if φ admits the integral representation

$$\varphi_m(\alpha) = \frac{1}{2}\int_\alpha^\infty (t-\alpha)^2 h(t)dt = \int_\alpha^\infty d\alpha \int_\alpha^\infty d\alpha \int_\alpha^\infty h(\alpha)\, d\alpha, \tag{56}$$

for some locally integrable function h in $L_1^{loc}(0,\infty)$ such that

$$\int_0^\infty t^2\,|h(t)|\,dt < \infty. \tag{57}$$

In fact $AC^3(0,\infty)$ is a generalization of the class of absolutely continuous functions on the half–axis. (For further discussions and results see [29], Chapter 2.)

Theorem 2 (Existence Part II)**.** *Let f satisfies the conditions of Theorem 1. If the fractional operator $\varphi_m(\alpha)$ belongs to the class $AC^3(0,\infty)$ for $m = 0,1,2$, then the Mehler–Fock transform $\mathcal{J}_m(q)$ satisfies the asymptotic behavior (48) and the equality (59), where for the case $m = 0$ we have to add the extra condition $\varphi_0'(0) = 0$.*

Proof. Substituting (56) into (54) and differentiating under the integral sign gives

$$\mathcal{J}_m(q) = \frac{1}{q}\int_0^\infty \sin\alpha q \int_\alpha^\infty (t-\alpha)h(t)\,dt\,d\alpha, \tag{58}$$

where the above iterated integral is absolutely convergent due to the fact

$$\int_0^\infty\int_\alpha^\infty (t-\alpha)|h(t)|dtd\alpha = \int_0^\infty |h(t)|\int_0^t (t-\alpha)d\alpha = \frac{1}{2}\int_0^\infty t^2|h(t)|\,dt < \infty.$$

Note that in the last inequality we have used condition (57). Now using Integration by parts twice in (58), assuming that $\varphi_m'(0) = \int_0^\infty th(t)\ dt = 0$, the estimates

$$\left|\int_\alpha^\infty (t-\alpha)h(t)dt\right| \le \int_\alpha^\infty t|h(t)|\,dt \le \frac{1}{\alpha}\int_1^\infty t^2|h(t)|dt \to 0, \quad \alpha\to\infty,$$
$$\int_\alpha^\infty |h(t)|dt \le \frac{1}{\alpha^2}\int_1^\infty t^2|h(t)|\,dt \to 0, \quad \alpha\to\infty,$$

imply

$$\mathcal{J}_m(q) = -\frac{1}{q^2}\int_0^\infty \cos\alpha q\int_\alpha^\infty h(t)\,dt = -\frac{1}{q^3}\int_0^\infty h(\alpha)\sin\alpha q\,d\alpha.$$

This proves (48) and (59) for cases $m = 0,1,2$ by noting that the equality $\varphi_m'(0) = 0$ indeed holds for all $m\in\mathbb{N}$ via (51). □

The Existence Theorems I and II have the following consequences. They play essential roles in the proof of Inversion Theorems.

Corollary 1 . *Under either of the assumptions of Theorem 1 for $m \geq 3$ or Theorem 2 for $m = 1, 2$, the following identity for the Mehler–Fock transform of oeredr m holds.*

$$\sqrt{\frac{2}{\pi}} \int_0^\infty q\mathcal{J}_m(q) \sin \alpha q \; dq = \frac{\sinh \alpha}{\Gamma(m - 1/2)} \int_\alpha^\infty \frac{f(\cosh \xi) \sinh^{1-m} \xi}{(\cosh \xi - \cosh \alpha)^{3/2-m}} \, d\xi, \;\; \alpha > 0. \tag{59}$$

Proof. Recall from the classical analysis (see [13]) that for an integrable function $f \in L_1(0, \infty)$ the sine Fourier transform

$$(F_s f)(\alpha) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(q) \sin \alpha q \, dq \tag{60}$$

exists and is well defined as a Lebesgue or Riemann improper integral. Moreover, as a consequence of the familiar Riemann–Lebesgue lemma, we have that $(F_s f)(\alpha)$ belongs to the space $C_0(0, \infty)$ satisfying the inverse sine Fourier transform formula,

$$f(q) = \sqrt{\frac{2}{\pi}} \int_0^\infty (F_s f)(\alpha) \sin \alpha q \, d\alpha. \tag{61}$$

Under either of the assumptions of Theorem 1 for $m \geq 3$ or Theorem 2 for $m = 1$ and 2, it follows immediately from the asymptotic result (48) that $q\mathcal{J}_m(q) \in L_1(0, \infty)$, and therefore the existence of the sine Fourier transform (60). Since for $m = 1, 2$, the identity (54) can be written in the form (51) as in the cases $m \geq 3$, it is straightforward to deduce (59) from (49), (51), and the inversion formula of the sine Fourier transform (61). (See [13] for more details and explanations.) □

Obviously for $m = 0$, as explained earlier, one can not in general differentiate under the integral sign in (54) and obtain (51). However, replacing (54) by (51) in the proof of the above corollary gives the following version of Corollary 1 for $m = 0$.

Corollary 2 . *Under the assumptions of Theorem 2 for $m = 0$, we have*

$$\int_0^\infty q\mathcal{J}_0(q) \sin \alpha q \; dq = -\frac{1}{\sqrt{2}} \frac{d}{d\alpha} \int_\alpha^\infty \frac{f(\cosh \xi) \sinh \xi}{(\cosh \xi - \cosh \alpha)^{1/2}} \, d\xi, \qquad \alpha > 0. \tag{62}$$

It should be mentioned that formula (62) serves as a starting point to invert the classical Mehler–Fock transformation by Sneddon's operational method. In fact, such a result has been recently proved in [30] (see Section 1.9), where one has imposed conditions on $\mathcal{J}_0(q)$. Our result for the inversion formula of the classical Mehler–Fock transform is based on conditions on f.

Theorem 3 (Inversion Theorem: Classical Case)**.** *If f satisfies the conditions of Theorem 1 for $m = 0$, then the classical Mehler–Fock transform $\mathcal{J}_0(q)$ admits the inversion formula*

$$f(\eta) = \int_0^\infty q \tanh \pi q \; P_{-\frac{1}{2}+iq}(\eta) \mathcal{J}_0(q) dq. \tag{63}$$

Proof. It is known (see [29]) that the identity

$$f(\cosh \xi) = -\frac{1}{\pi} \int_\xi^\infty \frac{1}{(\cosh \alpha - \cosh \xi)^{1/2}} \frac{d}{d\alpha} \int_\alpha^\infty \frac{f(\cosh u) \sinh u}{(\cosh u - \cosh \alpha)^{1/2}} du \; d\alpha \tag{64}$$

holds for any f such that the integral

$$\frac{d}{d\alpha} \int_\alpha^\infty \frac{f(\cosh u) \sinh u}{(\cosh u - \cosh \alpha)^{1/2}} du = \frac{\pi}{\sqrt{2}} \varphi_0'(\alpha),$$

where $\varphi(\alpha)$ defined as in (55), belongs to $L_1(0,\infty)$ and tends to 0 as $\alpha \to \infty$. Indeed, it follows from our assumption that

$$\begin{aligned}\int_0^\infty \left| \frac{d}{d\alpha} \int_\alpha^\infty \frac{f(\cosh u)\sinh u}{(\cosh u - \cosh\alpha)^{1/2}}\, du \right| d\alpha &= \frac{\pi}{\sqrt{2}} \int_0^\infty |\varphi_0'(\alpha)|\, d\alpha \\ &\le \frac{\pi}{\sqrt{2}} \int_0^\infty \int_\alpha^\infty (t-\alpha)|h(t)|\, dt\, d\alpha \\ &= \frac{\pi}{2\sqrt{2}} \int_0^\infty t^2 |h(t)| dt < \infty.\end{aligned}$$

Therefore (62) and (64) yield

$$f(\cosh\xi) = \frac{\sqrt{2}}{\pi} \int_\xi^\infty \frac{1}{(\cosh\alpha - \cosh\xi)^{1/2}} \int_0^\infty q\mathcal{J}_0(q) \sin\alpha q\, dq\, d\alpha. \tag{65}$$

Next we invert the order of integration in the left–hand side of (65) via Fubini's Theorem using the fact the function $(q,\alpha) \mapsto \dfrac{q\mathcal{J}_0(q)\sin\alpha q}{(\cosh\alpha - \cosh\xi)^{1/2}}$ belongs to the space $L_1\left((0,\infty)\times(\xi,\infty)\right)$ for all $\xi \ge 0$. Now, (63) follows from appealing to the value of the inner integral (see [15])

$$\frac{\sqrt{2}}{\pi} \int_\xi^\infty \frac{\sin\alpha q}{(\cosh\alpha - \cosh\xi)^{1/2}} d\alpha = \tanh\pi q\ P_{-\frac{1}{2}+iq}(\cosh\xi) \tag{66}$$

and making the obvious change of variable $\eta = \cosh\xi$. □

In order to invert the generalized Mehler–Fock transform of order $m \ge 1$, we reconsider the representation (59) assuming the imposed conditions in Theorem 1 and 2 for $m \ge 3$ and $m = 1, 2$, respectively. After an elementary change of variable one gets

$$\sqrt{\frac{2}{\pi}} \int_0^\infty q\mathcal{J}_m(q) \frac{\sin(q\ \mathrm{arccosh}\alpha)}{(\alpha^2-1)^{1/2}}\, dq = \frac{1}{\Gamma(m-1/2)} \int_\alpha^\infty \frac{f(\eta)(\eta^2-1)^{-m/2}}{(\eta-\alpha)^{3/2-m}}\, d\eta, \quad \alpha > 1. \tag{67}$$

Moreover, the following identity (see in [29], Chapter 1)

$$\begin{aligned}&\frac{(-1)^m}{\sqrt{\pi}\Gamma(m-1/2)} \frac{d^m}{d\eta^m} \int_\eta^\infty \frac{dt}{(t-\eta)^{1/2}} \int_t^\infty \frac{f(u)(u^2-1)^{-m/2}}{(u-t)^{3/2-m}} du \\ &\qquad = \frac{(-1)^m}{(m-1)!} \frac{d^m}{d\eta^m} \int_\eta^\infty (u-\eta)^{m-1} f(u)(u^2-1)^{-m/2}\, du \\ &\qquad = f(\eta)(\eta^2-1)^{-m/2}, \quad \eta > 1,\end{aligned} \tag{68}$$

holds for any $f \in L_1^{loc}(0,\infty)$ with the asymptotic behavior (46) and parameters a and b satisfying (47). Applying (68) to both sides of (67) implies

$$f(\eta)(\eta^2-1)^{-m/2} = \frac{(-1)^m\sqrt{2}}{\pi} \frac{d^m}{d\eta^m} \int_\eta^\infty \frac{dt}{(t^2-1)^{1/2}(t-\eta)^{1/2}} \int_0^\infty q\mathcal{J}_m(q) \sin(q\ \mathrm{arccosh}\ t)\, dq, \tag{69}$$

where $\eta > 1$. By a simple change of variables $t = \cosh\alpha$ and $\eta = \cosh\xi$, the right–hand side of (68) becomes

$$f(\cosh\xi)\sinh\xi^{-m} = \frac{(-1)^m\sqrt{2}}{\pi} \left(\frac{d}{d\cosh\xi}\right)^m \int_\xi^\infty \frac{d\alpha}{(\cosh\alpha - \cosh\xi)^{1/2}} \int_0^\infty q\mathcal{J}_m(q) \sin\alpha q\ dq. \tag{70}$$

Using Fubini's Theorem and employing the identity (66) with the variable η, one can write (70) in the form

$$f(\eta) = (-1)^m(\eta^2-1)^{m/2}\frac{d^m}{d\eta^m}\int_0^\infty q\tanh\pi q\ P_{-\frac{1}{2}+iq}(\eta)\mathcal{J}_m(q)dq,\ \ \eta>1, m\in\mathbb{N}_0, \tag{71}$$

Identity (71) is called the inversion formula for the generalized Mehler–Fock transform (33). Note that when $m=0$, formula (71) coincides formally with (63) proved in Theorem 3.

To rewrite (71) in the classical form (34); that is,

$$f(\eta) = (-1)^m\int_0^\infty q\tanh\pi q\ P^m_{-\frac{1}{2}+iq}(\eta)\mathcal{J}_m(q)dq, \tag{72}$$

one should obviously consider extra conditions under which it is possible to interchange differential– and integral operator in (70). Therefore, as we shall see shortly, the appearance of a set of new necessary conditions on f seems to be inevitable.

We start with the case $m=1$. Indeed, it is known that the uniform estimate

$$P^m_{-\frac{1}{2}+iq}(\eta) = O(q^{m-1/2}) \quad \text{as} \quad q\to\infty$$

holds for any compact set $K\subset\{\eta: 1\le\eta<\infty)$ (see [11], Theorem 1.8]). As a consequence of (48), we have $q^{3/2}\mathcal{J}_1(q)$ is integrable over $(0,\infty)$, which implies that the integral (71) is absolutely and uniformly convergent. As a consequence, one can differentiate inside the integral in (71) and obtain the classical inverse formula for $m=1$.

For $m=2,3,\ldots$, we employ the identity (see [21] formula 8.752)

$$P^m_{-\frac{1}{2}+iq}(\eta) = \frac{\Gamma(1/2+m+iq)}{\Gamma(1/2-m+iq)}P^{-m}_{-\frac{1}{2}+iq}(\eta). \tag{73}$$

Returning to (33), using (28) together with (A6) gives

$$\mathcal{J}_m(q) = \frac{\Gamma(1/2-m+iq)}{\Gamma(1/2+m+iq)}\int_1^\infty \frac{d^m}{d\eta^m}[P_{-\frac{1}{2}+iq}(\eta)](\eta^2-1)^{m/2}f(\eta)d\eta. \tag{74}$$

Next we apply the method of integration by parts m times in (74). In order to eliminate the free terms resulting from this procedure, we have to further assume that f belongs to $C^{(m)}(1,\infty)$ and satifies the conditions

$$\lim_{\eta\to1+}\frac{d^{n-1}}{d\eta^{n-1}}[(\eta^2-1)^{m/2}f(\eta)] = 0,\ \ n=1,\ldots,m, \tag{75}$$

and

$$\lim_{\eta\to\infty}\eta^{n-m-1/2}\frac{d^{n-1}}{d\eta^{n-1}}[(\eta^2-1)^{m/2}f(\eta)] = 0,\ \ n=1,\ldots,m, \tag{76}$$

In fact, the above conditions are direct consequences of the behavior of the conical functions near unity and infinity (see [21] 8.7–8.8). Now, m successive application of integration by parts in (29) gives

$$\mathcal{J}_m(q) = (-1)^m\frac{\Gamma(1/2-m+iq)}{\Gamma(1/2+m+iq)}\int_1^\infty P_{-\frac{1}{2}+iq}(\eta)\ \frac{d^m}{d\eta^m}[(\eta^2-1)^{m/2}f(\eta)]d\eta. \tag{77}$$

If we further assume that the integral

$$\int_1^\infty P_{-\frac{1}{2}}(\eta)\ \left|\frac{d^m}{d\eta^m}[(\eta^2-1)^{m/2}f(\eta)]\right| d\eta < \infty, \tag{78}$$

is finite, then one can estimate $|\mathcal{J}_m(q)|$ to get

$$|\mathcal{J}_m(q)| \le \left|\frac{\Gamma(1/2-m+iq)}{\Gamma(1/2+m+iq)}\right| \int_1^\infty P_{-\frac{1}{2}}(\eta)\ \left|\frac{d^m}{d\eta^m}[(\eta^2-1)^{m/2}f(\eta)]\right| d\eta < C\, q^{-2m},\ q\to\infty, \tag{79}$$

where C is a constant and in the last inequalty we have applied the Stirling asymptotic formula for the ratio of gamma functions (see fo example [21] formula 8.327). The estimate (79) is what we need at last. It implies $q^{m+1/2}\mathcal{J}_m(q) \in L_1(0,\infty)$ for and, as a result, formula (72) holds for $m = 2, 3, \ldots$, as well since one can now differentiate under the integral (71) via its absolute and uniform convergence. We summarize the above result in the last theorem of this section.

Theorem 4 (Inversion Theorem Part II)**.** *Let $f \in C^{(m)}(1,\infty)$ and $m \in \mathbb{N}$. Suppose f satisfies either the assumptions of Theorem 1 for $m \ge 3$ or those of Theorem 2 for $m = 1, 2$. If we further assume the conditions (75), (76), and (78), then generalized Mehler–Fock transform* (1) *admits for all $\eta \ge 1$ the inversion formula (72) given by*

$$f(\eta) = (-1)^m \int_0^\infty q\tanh\pi q\ P^m_{-\frac{1}{2}+iq}(\eta)\mathcal{J}_m(q)dq.$$

Before closing this section, we make one final remark. As it has already surfaced in the argument leading to the proof of Theorem 4, we did not need any extra assumptions on f for the case $m = 1$. However, in most applications, one needs the inversion formula (72) for all $m \ge 1$. Therefore, we have stated the theorem for all $m \in \mathbb{N}$ and have not treated $m = 1$ seperately.

2. Example

In this section we treat an example of the generalized Mehler–Fock transform (33), which are important for applications. Recall from (44) that the function $f(\eta) = e^{-\gamma\eta}$, where $\gamma > 0$, has the classical Mehler–Fock transform; i.e., (33) with $m = 0$,

$$\mathcal{J}_0(q) = \int_1^\infty e^{-\gamma\eta}P_{-\frac{1}{2}+iq}(\eta)\, d\eta = \sqrt{\frac{2}{\pi\gamma}}K_{iq}(\gamma), \tag{80}$$

where, as discussed in (45), $K_{iq}(\gamma)$ is the modified Bessel function and it represents the kernel of the Kontorovich–Lebedev transform (see [11]). This result can be generalized for $m \in \mathbb{N}$ by considering

$$f(\eta) = e^{-\gamma\eta}(\eta^2-1)^{m/2}.$$

In fact, using relation (2.17.7.1) in [22] we get

$$\int_1^\infty e^{-\gamma\eta}(\eta^2-1)^{m/2}P^{-m}_{-\frac{1}{2}+iq}(\eta)\, d\eta = \sqrt{\frac{2}{\pi}}\gamma^{-m-1/2}K_{iq}(\gamma). \tag{81}$$

However, the latter transformation slightly generalizes (33) and coincides with $\mathcal{J}_m(q)$ only for $m = 0$. Our goal is to calculate the generalized Mehler–Fock transform (33) of the function $e^{-\gamma\eta}$, which as far as the authors are aware of, is absent in the reference books. It should also be mentioned that

we only treat the case where n is an even integer. The reason is that it is technically very difficult to express the Mehler–Fock transforms of $e^{-\gamma\eta}$ of odd order in terms of suitable special functions.

So let m be an even number, i.e. $m = 2n,\ n \in \mathbb{N}$. Then the corresponding Mehler–Fock transform (33) becomes

$$\begin{aligned}\mathcal{J}_{2n}(q) &= \frac{\Gamma(1/2-2n+iq)}{\Gamma(1/2+2n+iq)}\int_1^\infty \frac{d^{2n}}{d\eta^{2n}}[P_{-\frac{1}{2}+iq}(\eta)](\eta^2-1)^n e^{-\gamma\eta}\,d\eta \\ &= \frac{\Gamma(1/2-2n+iq)}{\Gamma(1/2+2n+iq)}\sum_{k=0}^{n}(-1)^{n-k}\binom{n}{k}\int_1^\infty \frac{d^{2n}}{d\eta^{2n}}[P_{-\frac{1}{2}+iq}(\eta)]\eta^{2k}e^{-\gamma\eta}\,d\eta.\end{aligned} \tag{82}$$

Using the method of integration by parts in (82) together with (73) and (B6), and the asymptotic behavior of the conical functions near unity [21] given by

$$\lim_{\eta\to 1+}\frac{d^l}{d\eta^l}[P_{-\frac{1}{2}+iq}(\eta)] = \frac{\Gamma(1/2+l+iq)}{\Gamma(1/2-l+iq)\ 2^l\ l!}, l = 0,1,\ldots,2n-1$$

one can deduce from equality (80) that

$$\begin{aligned}\int_1^\infty \frac{d^{2n}}{d\eta^{2n}}[P_{-\frac{1}{2}+iq}(\eta)]\eta^{2k}e^{-\gamma\eta}d\eta &= \sqrt{\frac{2}{\pi}}\frac{d^{2k}}{d\gamma^{2k}}\left(\gamma^{2n-1/2}K_{iq}(\gamma)\right) \\ &\quad - \sum_{l=0}^{2n-1}\frac{\Gamma(iq+2n-l-1/2)}{\Gamma(iq-2n+l+3/2)}\frac{2^{-(2n-l-1)}}{(2n-l-1)!}\frac{d^{2k}}{d\gamma^{2k}}\left(\gamma^l e^{-\gamma}\right).\end{aligned} \tag{83}$$

Substituting (83) into (36) we obtain the generalized Mehler–Fock transform (33) of the function $e^{-\gamma\eta}$ for even $m = 2n$, given by

$$\begin{aligned}\mathcal{J}_{2n}(q) = (-1)^n\frac{\Gamma(1/2-2n+iq)}{\Gamma(1/2+2n+iq)}&\left[\sum_{l=0}^{2n-1}\sum_{k=0}^{n}(-1)^{k+1}\binom{n}{k}\frac{\Gamma(iq+2n-l-1/2)}{\Gamma(iq-2n+l+3/2)}\right. \\ &\left.\times\frac{2^{-(2n-l-1)}}{(2n-l-1)!}\frac{d^{2k}}{d\gamma^{2k}}\left(\gamma^l e^{-\gamma}\right) + \sqrt{\frac{2}{\pi}}\sum_{k=0}^{n}(-1)^k\binom{n}{k}\frac{d^{2k}}{d\gamma^{2k}}\left(\gamma^{2n-1/2}K_{iq}(\gamma)\right)\right].\end{aligned} \tag{84}$$

Also note that when $m = 0$, equality (84) becomes (80) as expected.

III. THE CONICAL CASE

In many SPM applications, a cone may be considered as a special case of a very sharp hyperboloid. It is understood that, from the current manufacturing point of view, the degree of curvature for a conical probe will be scale-dependent. For example, a perfectly conical probe at the micrometer scale will indeed be a hyperboloidal (or with other geometries) probe at the nanometer scale. However, atomically sharp probes have been produced for applications in SPM. Also, powerful numerical techniques, such as finite elements, are routinely used to compute the potential and field distributions in geometries such as treated here. The aim of this section is the use of functions with fractional index, where Mehler-Fock transforms may find potential applications.

A. The boundary value problem

In the case of a conical model for the probe as shown in Fig. 9, working in spherical coordinates, the particular solution to Laplace's equation is separated as

$$\Phi(\mathbf{r}) = h_m(\varphi)\, t_\nu^m(r)\, u_\nu^m(\theta).$$

Assuming a constant (tensor) ϵ, it can be shown (see Section II) that the general solution to the boundary value problem (18)–(21) is given by

$$\Phi(\mathbf{r}) = \sum_{m=0}^{\infty} \frac{h_m(\varphi)}{\sqrt{r}} \int_0^\infty u_q^m(\cos\theta) w_q^m(r)\, dq, \tag{85}$$

where, as in the case of prolate spheroidal system in subsection D of Section II, $h_m(\varphi)$ is given by (14) and from equality (27)

$$u_q^m(\cos\theta) = D_q^m \times \begin{cases} \alpha(\epsilon) P^m_{-\frac{1}{2}+iq}(\cos\theta) + P^m_{-\frac{1}{2}+iq}(-\cos\theta) & : \Omega_I \\ \beta(\epsilon) P^m_{-\frac{1}{2}+iq}(-\cos\theta) & : \Omega_{II}, \end{cases} \tag{86}$$

where

$$\alpha(\epsilon) = \frac{\epsilon_I - \epsilon_{II}}{\epsilon_I + \epsilon_{II}}, \qquad \beta(\epsilon) = \frac{2\epsilon_I}{\epsilon_I + \epsilon_{II}}, \tag{87}$$

and

$$w_q^m = \sqrt{r} t_q^m = A_q^m \cos(q \ln r) + B_q^m \sin(q \ln r). \tag{88}$$

Absorbing D_q^m from (86) in A_q^m and B_q^m in equation (88) , satisfaction of the boundary condition at the probe requires $f(r,\varphi) = \Phi(r, \theta_t, \varphi)$, which after an integration in φ and setting

$$g(r) = \sqrt{r} \int f(r,\varphi)\, d\varphi$$

results in

$$g(r) = \sum_{m=0}^{\infty} \int_{\varphi_1}^{\varphi_2} h_m(\varphi) \int_0^\infty dq\, u_q^m(\cos\theta_t) w_q^m(r). \tag{89}$$

Now assuming g is a good function, it can be expanded in a Fourier integral

$$g(r) = \sqrt{r} \int_{\varphi_1}^{\varphi_2} f(r,\varphi)\, d\varphi = \int_0^\infty dq\, [\mathcal{C}_q \cos(q \ln r) + \mathcal{S}_q \sin(q \ln r)], \tag{90}$$

with

$$\begin{aligned} \mathcal{C}_q &= \frac{1}{\pi} \int_0^\infty \frac{1}{r}\, g(r) \cos(q \ln r)\, dr \\ \mathcal{S}_q &= \frac{1}{\pi} \int_0^\infty \frac{1}{r}\, g(r) \sin(q \ln r)\, dr. \end{aligned} \tag{91}$$

Therefore

$$\begin{aligned}\mathcal{C}_q &= \sum_{m=0}^{\infty} u_q^m(\cos\theta_t) A_q^m \int_{\varphi_1}^{\varphi_2} h_m(\varphi)\, d\varphi,\\ \mathcal{S}_q &= \sum_{m=0}^{\infty} u_q^m(\cos\theta_t) B_q^m \int_{\varphi_1}^{\varphi_2} h_m(\varphi)\, d\varphi.\end{aligned} \tag{92}$$

Thus, although the boundary function f does not have to be φ symmetric, it must be defined on the closed φ interval. For $\varphi_1 = 0$, and $\varphi_2 = 2\pi$ we obtain

$$\begin{aligned}A_q^m &= \frac{\delta_m^0 \mathcal{C}_q}{u_q^m(\cos\theta_t)},\\ B_q^m &= \frac{\delta_m^0 \mathcal{S}_q}{u_q^m(\cos\theta_t)}.\end{aligned} \tag{93}$$

Before studying a specific form of the boundary function f, we recuperate the potential

$$\Phi(\mathbf{r}) = \frac{1}{\sqrt{r}} \int_0^{\infty} \frac{v_q^0(\cos\theta)}{v_q^0(\cos\theta_t)} \left[\mathcal{C}_q \cos(q\ln r) + \mathcal{S}_q \sin(q\ln r)\right] dq, \tag{94}$$

where $\mathcal{C}_q$ and $\mathcal{S}_q$ are given by the integrals (91),

$$v_q^0(\cos\theta) = \begin{cases} \alpha(\epsilon) P_{-\frac{1}{2}+iq}(\cos\theta) + P_{-\frac{1}{2}+iq}(-\cos\theta) & : \Omega_I \\ \beta(\epsilon) P_{-\frac{1}{2}+iq}(-\cos\theta) & : \Omega_{II}, \end{cases} \tag{95}$$

and

$$v_q^0(\cos\theta_t) = \alpha(\epsilon) P_{-\frac{1}{2}+iq}(\cos\theta_t) + P_{-\frac{1}{2}+iq}(-\cos\theta_t).$$

B. Examples

In this section we consider two examples of the boundary function which are important in applications. As our first example, let the boundary function $f(r,\varphi)$ be axially symmetric in φ and behave like Fermi–Dirac distribution in r; that is,

$$f(r) = \frac{V_0}{e^{(r-r_0)/\gamma} + 1}, \tag{96}$$

where r_0 is a cut–off radius and γ is a constant. It follows that the potential is continuous on $[0,\infty)$ and is of bounded variation in every finite variation $0 < r_1 < r_2 < \infty$. Thus we can calculate the functions $\mathcal{C}_q$ and $\mathcal{S}_q$ from (91). Letting

$$\mathcal{D}_q = \mathcal{C}_q + i\mathcal{S}_q,$$

it follows from the equations (91) that

$$\begin{aligned}\mathcal{D}_q &= \frac{1}{\pi}(\varphi_2 - \varphi_1) \int_0^{\infty} \frac{V_0}{e^{(r-r_0)/\gamma} + 1} r^{-\frac{1}{2}} e^{iq\ln r}\, dr\\ &= \frac{V_0}{\pi}(\varphi_2 - \varphi_1) \int_0^{\infty} \frac{1}{e^{(r-r_0)/\gamma} + 1} r^{s-1}\, dr,\end{aligned} \tag{97}$$

where $s = \frac{1}{2} + iq$. Now since

$$\frac{1}{e^{(r-r_0)/\gamma}+1} = \begin{cases} 1 - \sum_{n=0}^{\infty}(-1)^n e^{\frac{1}{\gamma}(n+1)(r-r_0)} & r \le r_0 \\ \sum_{n=0}^{\infty}(-1)^n e^{-\frac{1}{\gamma}(n+1)(r-r_0)} & r > r_0, \end{cases}$$

one can use the uniform convergence argument to obtain

$$\begin{aligned} I_q &= \Big(\int_0^{r_0} + \int_{r_0}^{\infty}\Big)\frac{1}{e^{(r-r_0)/\gamma}+1} r^{s-1}\,dr \\ &= \frac{1}{s}r_0^s - \sum_{n=0}^{\infty}(-1)^n \int_0^{r_0} e^{\frac{1}{\gamma}(n+1)(r-r_0)} r^{s-1}\,dr + \sum_{n=0}^{\infty}(-1)^n \int_{r_0}^{\infty} e^{-\frac{1}{\gamma}(n+1)(r-r_0)} r^{s-1}\,dr \end{aligned}$$

Now rewriting the last integral as $\int_{r_0}^{\infty} = \int_0^{\infty} - \int_0^{r_0}$, we get

$$\begin{aligned} I_q = \frac{1}{s}r_0^s - \sum_{n=0}^{\infty}(-1)^n \int_0^{r_0} \Big(e^{-\frac{1}{\gamma}(n+1)(r-r_0)} + e^{\frac{1}{\gamma}(n+1)(r-r_0)}\Big) r^{s-1}\,dr \\ + \sum_{n=0}^{\infty}(-1)^n e^{\frac{1}{\gamma}(n+1)r_0} \int_0^{\infty} e^{-\frac{1}{\gamma}(n+1)r} r^{s-1}\,dr. \end{aligned} \tag{98}$$

The last integral in the above equality (see for example [12], p. 610, no. 4) is the Mellin transform of the function e^{-ar} given by

$$\int_0^{\infty} e^{-\frac{1}{\gamma}(n+1)r} r^{s-1}\,dr = \frac{\gamma^s}{(n+1)^s}\Gamma(s). \tag{99}$$

A simple change of variable gives

$$\int_0^{r_0} e^{-a(r-r_0)} r^{s-1}\,dr = \int_0^{r_0} e^{ar}(r_0-r)^{s-1}\,dr \tag{100}$$

The last integral is a fractional integrals of Riemann–Louisville type (see [12], p. 605, no. 3) given by

$$\int_0^{r_0} e^{ar}(r_0-r)^{s-1}\,dr = \frac{1}{s}r_0^s\, {}_1F_1(1; s+1; ar_0), \tag{101}$$

where ${}_1F_1(s; s+1; ar_0)$, denotes the generalized hypergeometric function (see [12] p. 49). Finally, using (99) and (101) we get

$$\begin{aligned} I_q = \frac{1}{s}r_0^s - \frac{1}{s}r_0^s \sum_{n=0}^{\infty}(-1)^n \Big({}_1F_1(1; s+1; \tfrac{-1}{\gamma}(n+1)r_0) + {}_1F_1(1; s+1; \tfrac{1}{\gamma}(n+1)r_0)\Big) \\ + \gamma^s\Gamma(s)\sum_{n=0}^{\infty}(-1)^n \frac{e^{(n+1)r_0/\gamma}}{(n+1)^s}, \end{aligned} \tag{102}$$

where $s = \frac{1}{2} + iq$. Now C_q and S_q can be computed by taking the real and imaginary parts of I_q respectively. Note that (102) represents the Mellin transform of $(Ae^{ar}+1)^{-1}$, where $A = e^{-r_0/\gamma}$. More precisely

$$I_q = \mathcal{M}\Big(\frac{1}{e^{(r-r_0)/\gamma}+1}\Big)(\frac{1}{2} + iq), \tag{103}$$

where, as mentioned, $\mathcal{M}$ stands for the Mellin transform defined by

$$\mathcal{M}(f)(s) = \int_0^\infty f(r) r^{s-1}\, dr, \tag{104}$$

for any f such that the above integral exists for at least one value s_0 of s. (See [21] p. 1129 or [12] p. 201.) It is also worth mentioning that, as far as the authors know, in the literature there is only the Mellin transform of $(e^{ar}+1)^{-1}$ with $a > 0$.

As the second example, we examine a Heaviside–like boundary function

$$f(r) = \begin{cases} V_0 & : \quad 0 < r < r_0 \\ 0 & : \quad r > r_0. \end{cases} \tag{105}$$

Similar to the first example, we let

$$\mathcal{D}_q = \mathcal{C}_q + i\mathcal{S}_q.$$

Then equations (91) together with (104) imply

$$\mathcal{D}_q = \frac{V_0}{\pi}(\varphi_2 - \varphi_1) \int_0^{r_0} r^{s-1}\, dr = \frac{V_0}{\pi s}(\varphi_2 - \varphi_1){r_0}^s. \tag{106}$$

where $s = \frac{1}{2} + iq$. Taking real and imaginary parts, we have

$$\begin{aligned} \mathcal{C}_q &= \frac{\sqrt{r_0}}{\pi\sqrt{1+4q^2}}\Big(\cos(q\ln r_0) + 2q\sin(q\ln r_0)\Big) \\ \mathcal{S}_q &= \frac{\sqrt{r_0}}{\pi\sqrt{1+4q^2}}\Big(\sin(q\ln r_0) - 2q\cos(q\ln r_0)\Big). \end{aligned} \tag{107}$$

IV. CONCLUSIONS

Nanoscience is generally regarded as highly cross-disiplineary. We presented a rather general motivation for the use of index transforms of the Mehler-Fock kind, and special functions with fractional index such as conical functions in modeling problems relevant to nanoscience. While our presentation primarily targeted the solutions to the Laplace equation in hyperboloidal and conical domains, the main results of the forward and inverse Mehler-Fock transform may be applied to other problems that lend themselves to modeling in these geometries. Furthermore, for Laplace's equation in hyperboloidal geometry, the nature of the eigenvalues were discussed, as these are closely related to the surface modes of the modeled structures. The examples treated demonstrate how experimentally realistic potential distributions on a hyperboloidal probe may be tackled with the general form of the Mehler-Fock transform. Index transforms such as presented here appear to have stayed aloof from modeling of nanostructures. The presented material can therefore open new venues in the investigation of nanostructure modeling. Optical, electronic, and mechanical response of many structures can be advantageously investigated in the spheroidal geometry following the results here.

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APPENDIX A

As an example of a modeling domain consider the region Ω defined by:

$$\Omega = \{(x(\zeta,\theta,\varphi), y(\zeta,\theta,\varphi)) : \zeta \in [0, 2.5] \wedge \theta \in [0,\pi] \wedge \varphi = 0\},$$

and displayed in Fig. 6. Thus, fixing θ or $\mu = \mu_c$ yields the surface of a hyperboloid of revolution with a boundary in the xz–plane presented by:

$$(x, z) = z_0 \left(\sqrt{(\eta^2 - 1)(1 - \mu_c^2)}\,,\, \eta\mu_c\right),$$

which can easily be rearranged to give:

$$\left(\frac{z}{\mu_c}\right)^2 - \left(\frac{x}{\sqrt{1-\mu_c^2}}\right)^2 = z_0^2, \tag{A1}$$

or

$$z(x) = \pm z_0\mu_c\sqrt{1 + \frac{x^2}{z_0^2\,(1-\mu_c^2)}}, \tag{A2}$$

which represents in xz plane two symmetrical hyperboloids with focal points $z = \pm z_0$. Similarly equation (4) maps, for fixed ζ or $\eta = \eta_c$, the surface of an ellipsoid with a trace in the xz–plane given by:

$$\left(\frac{z}{\eta_c}\right)^2 + \left(\frac{x}{\sqrt{\eta_c^2 - 1}}\right)^2 = z_0^2,$$

or

$$z(x) = \pm z_0\eta_c\sqrt{1 - \frac{x^2}{z_0^2\,(\eta_c^2-1)}},$$

which represents in the xz–plane the contour of an ellipsoid with focal length z_0.

From equation (A1) we get the inverse transformation to (4) as:

$$\begin{aligned}
\eta &= \left[\frac{1}{2}\left(1 + \frac{R^2}{z_0^2}\right) + \sqrt{\frac{1}{4}\left(1 + \frac{R^2}{z_0^2} - \frac{z_2}{z_0^2}\right)}\right]^{\frac{1}{2}}, \\
\mu &= \pm\left[\frac{1}{2}\left(1 + \frac{R^2}{z_0^2}\right) - \sqrt{\frac{1}{4}\left(1 + \frac{R^2}{z_0^2} - \frac{z_2}{z_0^2}\right)}\right]^{\frac{1}{2}}, \\
\varphi &= \arctan\left(\frac{y}{x}\right),
\end{aligned} \tag{A3}$$

where $R = \sqrt{x^2 + y^2}$, which for a particular hyperboloid $\theta = \theta_t$ is written as:

$$R = z_0 \sin\theta_t \sqrt{\eta^2 - 1}. \tag{A4}$$

From the transformation properties of (4) one can derive the metric coefficients for the spheroidal system as:

$$\mathbf{g} = \begin{pmatrix} g_{11} & 0 & 0 \\ 0 & g_{22} & 0 \\ 0 & 0 & g_{33} \end{pmatrix} = z_0^2 \begin{pmatrix} \dfrac{\eta^2-\mu^2}{\eta^2-1} & 0 & 0 \\ 0 & \dfrac{\eta^2-\mu^2}{1-\mu^2} & 0 \\ 0 & 0 & (\eta^2-1)(1-\mu^2) \end{pmatrix}, \tag{A5}$$

with the surface element of a hyperboloid as:

$$dA_2 = \sqrt{g_{11}g_{33}}\, d\eta d\varphi, \tag{A6}$$

which using (A5) gives:

$$dA_\mu = z_0^2 \sqrt{(\eta^2-\mu^2)(1-\mu^2)}\, d\eta d\varphi. \tag{A7}$$

Integrating the differential surface element (A7) over an arbitrary and finite region of the hyperboloid $\mu = \mu_t$, and $1 \le \eta \le \eta_0$ we get:

$$A(\eta_0, \mu_t) = \pi z_0^2 \sqrt{1-\mu_t^2} \left[\eta_0 \sqrt{\eta_0^2 - \mu_t^2} - \sqrt{1-\mu_t^2} + \mu_t^2 \ln\left(\frac{1+\sqrt{1-\mu_t^2}}{\eta_0 + \sqrt{\eta_0^2-\mu_t^2}} \right) \right], \tag{A8}$$

which can be used for averaging purposes.

Expressing the unit vectors in terms of Cartesian unit vectors:

$$\begin{aligned} \bar{e}_i &= \frac{1}{\sqrt{g_{ii}}} \frac{\partial \bar{r}}{\partial u_i} \\ &= \frac{1}{\sqrt{g_{ii}}} \frac{\partial}{\partial u_i} \left[z_0 \sqrt{(\eta^2-1)(1-\mu^2)} (\cos\varphi \bar{e}_x + \sin\varphi \bar{e}_y) + z_0 \eta \mu \bar{e}_z \right], \quad i = 1,2,3, \end{aligned} \tag{A9}$$

yields the following orthogonal unit vectors for spheroidal unit vectors:

$$\begin{aligned} \bar{e}_\eta(\eta,\mu,\varphi) &= \sqrt{\frac{\eta^2-1}{\eta^2-\mu^2}} \left[\mu \bar{e}_z + \frac{\eta\left(1-\mu^2\right)}{\sqrt{(\eta^2-1)(1-\mu^2)}} (\cos\varphi \bar{e}_x + \sin\varphi \bar{e}_y) \right], \\ \bar{e}_\mu(\eta,\mu,\varphi) &= \sqrt{\frac{1-\mu^2}{\eta^2-\mu^2}} \left[\eta \bar{e}_z - \frac{\mu\left(\eta^2-1\right)}{\sqrt{(\eta^2-1)(1-\mu^2)}} (\cos\varphi \bar{e}_x + \sin\varphi \bar{e}_y) \right], \\ \bar{e}_\varphi(\eta,\mu,\varphi) &= \left[-\sin\varphi \bar{e}_x + \cos\varphi \bar{e}_y \right], \end{aligned} \tag{A10}$$

as shown in Fig. 7. The unit vector $\bar{e}_\eta$ points in the direction of the tangent to the hyperboloid at the crossing point with the corresponding spheroid and perpendicular to $\bar{e}_\mu$ which is parallel to a tangent of the spheroid. Noting the special cases:

$$\begin{aligned} \bar{e}_\eta(\eta,0,0) &= \bar{e}_x, \\ \bar{e}_\mu(\eta,0,0) &= \bar{e}_z, \end{aligned} \tag{A11}$$

appropriate for transition between the hyperboloidal and Cartesian boundaries.

The Laplacian in this coordinate system is easily derived from the general expression for ∇^2 in curvilinear coordinates:

$$\nabla^2 = \frac{1}{\sqrt{g}} \sum_i \frac{\partial}{\partial x_i} \left(\frac{\sqrt{g}}{g_{ii}} \frac{\partial}{\partial x_i} \right), \quad i = 1, 2, 3, \tag{A12}$$

where $g = |\mathbf{g}|$. Using (A5) and (A12), the Laplacian reads:

$$\nabla^2 = \frac{1}{z_0^2(\eta^2 - \mu^2)} \left(\frac{\partial}{\partial \eta} \left[(\eta^2 - 1) \frac{\partial}{\partial \eta} \right] + \frac{\partial}{\partial \mu} \left[(1 - \mu^2) \frac{\partial}{\partial \mu} \right] + \left[\frac{1}{1 - \mu^2} + \frac{1}{\eta^2 - 1} \right] \frac{\partial^2}{\partial \varphi^2} \right). \tag{A13}$$

APPENDIX B

$$P^m_{-\frac{1}{2}+iq}(\cos\theta) = (-1)^m \frac{2^{m+\frac{1}{2}}}{\pi(2m-1)!!} \frac{1}{\sin^m\theta} \frac{\Gamma(\frac{1}{2}+m+iq)}{\Gamma(\frac{1}{2}-m+iq)} \int_0^\theta \frac{\cosh qx}{(\cos x - \cos\theta)^{\frac{1}{2}-m}} \tag{B1}$$

$$|P^m_{-\frac{1}{2}+iq}(x)| \leq \left(\frac{\sqrt{x^2+1}}{x+1} \right)^m \frac{\Gamma(m+1/2)}{\Gamma(1/2)} \cosh \pi q P^0_{-\frac{1}{2}}(x) \tag{B2}$$

$$\frac{P^0_{-\frac{1}{2}+iq}(\cos\theta)}{P^0_{-\frac{1}{2}+iq}(\cos\theta_t)} \leq 1, \qquad 0 \leq \theta \leq \theta_t \tag{B3}$$

$$\frac{2\pi}{\cosh \pi q} \left[P_{-\frac{1}{2}+iq}(0) \right]^2 = \int_0^\infty \frac{d\eta}{\sqrt{\eta^2+1}} \left[P^0_{-\frac{1}{2}+iq}(i\eta) + P^0_{-\frac{1}{2}+iq}(-i\eta) \right] \tag{B4}$$

From these integral representations and the definition of Z^m_q, one can easily deduce that

$$P^m_{-\frac{1}{2}+iq}(z) = P^m_{-\frac{1}{2}-iq}(z).$$

An integral representation appropriate for numerical evaluation of these functions can be obtained by considering the following substitution :

$$x = 2 \arcsin \left(\sin y \sin \frac{\theta}{2} \right),$$

which transforms the integration region in (B1) as

$$x = 0 \to y = 0, \quad \text{and} \quad x = \theta \to y = \frac{\pi}{2},$$

Since

$$dx = \frac{2 \cos y \sin \frac{\theta}{2}}{\sqrt{1 - \sin^2 y \sin^2 \frac{\theta}{2}}} dy,$$

$$\cos x = 1 - 2 \sin^2 y \sin^2 \frac{\theta}{2},$$

we arrive at the result by Kölbig [31].

Van Nostrand [32] derives the following orthogonality relation for the conical functions with argument $1 \leq \eta < \infty$:

$$\int_1^\infty P^m_{-\frac{1}{2}+iq}(\eta) P^m_{-\frac{1}{2}+iq'}(\eta)\, d\eta = \frac{Z^m_q}{q \tanh \pi q} \delta(q - q'), \tag{B5}$$

The conical functions of higher azimuthal order can be generated by successive differentiations of the zero order function:

$$\begin{aligned} P^m_{-\frac{1}{2}+iq}(\mu) &= (-1)^m (1-\mu^2)^{m/2} \frac{d^m P^0_{-\frac{1}{2}+iq}(\mu)}{d\mu^m}, \\ P^m_{-\frac{1}{2}+iq}(\eta) &= (\eta^2 - 1)^{m/2} \frac{d^m P^0_{-\frac{1}{2}+iq}(\eta)}{d\eta^m}. \end{aligned} \tag{B6}$$

In writing equations (B6), we have adopted the sign convention of references [21] and [33], as opposed to the alternative convention that does not include $(-1)^m$ term. From equation (B6) we can derive the following:

$$\frac{dP^m_{-\frac{1}{2}+iq}(\pm\mu)}{d\mu} = \frac{-m\mu}{1-\mu^2} P^m_{-\frac{1}{2}+iq}(\pm\mu) \mp \frac{P_{-\frac{1}{2}+iq}(\pm\mu)}{\sqrt{1-\mu^2}} \tag{B7}$$

where the negative argument relation results upon $\theta \to \theta - \pi$. Similarly

$$\frac{dP^m_{-\frac{1}{2}+iq}(\eta)}{d\eta} = \frac{m\eta}{\eta^2 - 1} P^m_{-\frac{1}{2}+iq}(\eta) + \frac{P_{-\frac{1}{2}+iq}(\eta)}{\sqrt{\eta^2 - 1}} \tag{B8}$$

from these relations we can easily derive the necessary recursion relations, which have been used to evaluate the higher order functions as the explicit evaluation of these functions, for higher $m \neq 0, 1$, using an integral representation becomes less effective. This deterioration was observed by Wronskian check. Evaluating (B7) for $\mu \to 0$, gives

$$\left. \frac{dP^m_{-\frac{1}{2}+iq}(\mu)}{d\mu} \right|_{\mu-0} = \left. \frac{dP^m_{-\frac{1}{2}+iq}(-\mu)}{d\mu} \right|_{\mu-0}. \tag{B9}$$

The following Wronskian defined for functions with argument μ:

$$\begin{aligned} W^m_q &= P^m_{-\frac{1}{2}+iq}(\mu) \frac{dP^m_{-\frac{1}{2}+iq}(-\mu)}{d\mu} - P^m_{-\frac{1}{2}+iq}(-\mu) \frac{dP^m_{-\frac{1}{2}+iq}(\mu)}{d\mu} \\ &= \frac{2 Z^m_q \cosh \pi q}{\pi \sqrt{1-\mu^2}}, \end{aligned} \tag{B10}$$

will be used to check the precision of the numerical evaluation of $P^m_{-\frac{1}{2}+iq}(\mu)$.

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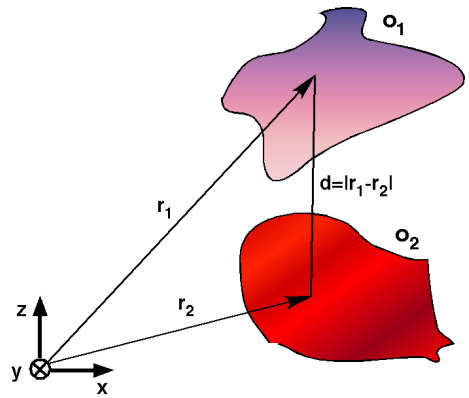

FIG. 1: In the macroscopic picture, the effect of forces become measurable at small distances $d = |\mathbf{r_1} - \mathbf{r_2}|$ between the two objects $\mathbf{O_1}$ and $\mathbf{O_2}$. Such force exchange allows $\mathbf{O_1}$ to probe $\mathbf{O_2}$ or vice versa.

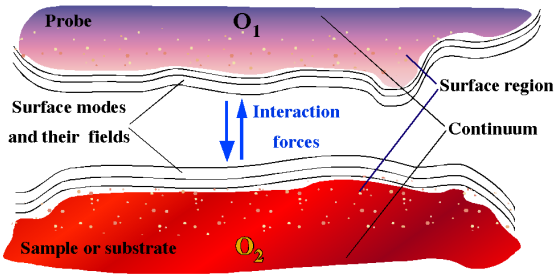

FIG. 2: In the microscopic picture, at small $d \propto 10^{-9}$ m, the atomic structure in the surface region of the two objects $\mathbf{O_1}$ and $\mathbf{O_2}$ become important. Surface modes find many applications in the submicrometer realm.

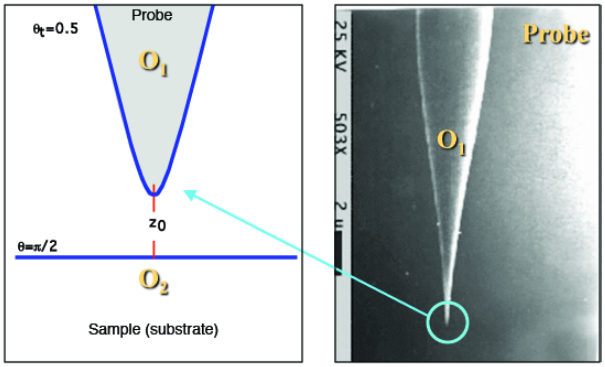

FIG. 3: Modeling based on an image of a SPM probe (right) in spheroidal geometry by a one-sheeted hyperboloid (left).

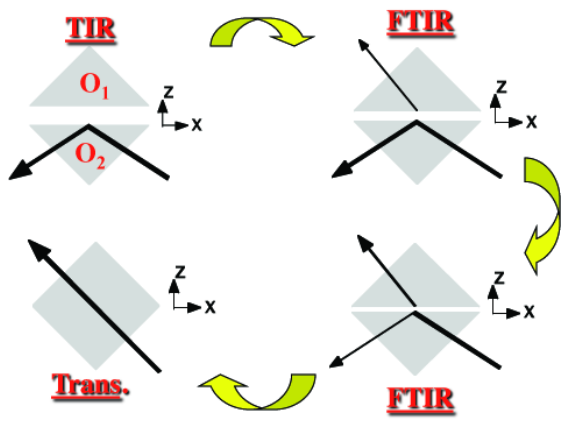

FIG. 4: Tunneling at small $|\mathbf{r_1} - \mathbf{r_2}|$: Light propagating (indicated by the black arrow) initially in medium $\mathbf{O_1}$ only tunnels to $\mathbf{O_2}$ when $|\mathbf{r_1} - \mathbf{r_2}| \propto \lambda$, and increase to full transmission for $|\mathbf{r_1} - \mathbf{r_2}| \to 0$. The processes of total internal reflection (TIR) and frustrated total internal reflection (FTIR), and the final full transmission are shown.

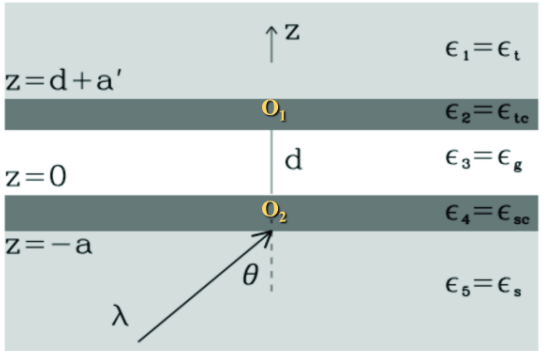

FIG. 5: Cartesian tunneling geometry with a finite gap d but an infinite extent $z \to \pm\infty$. A photon of wavelength λ incident at an angle θ propagates from $\mathbf{O_2}$ to $\mathbf{O_1}$ by tunneling. The $\epsilon_i, i = 1-5$ characterizes the different media involved, and a, and a' are the thicknesses.

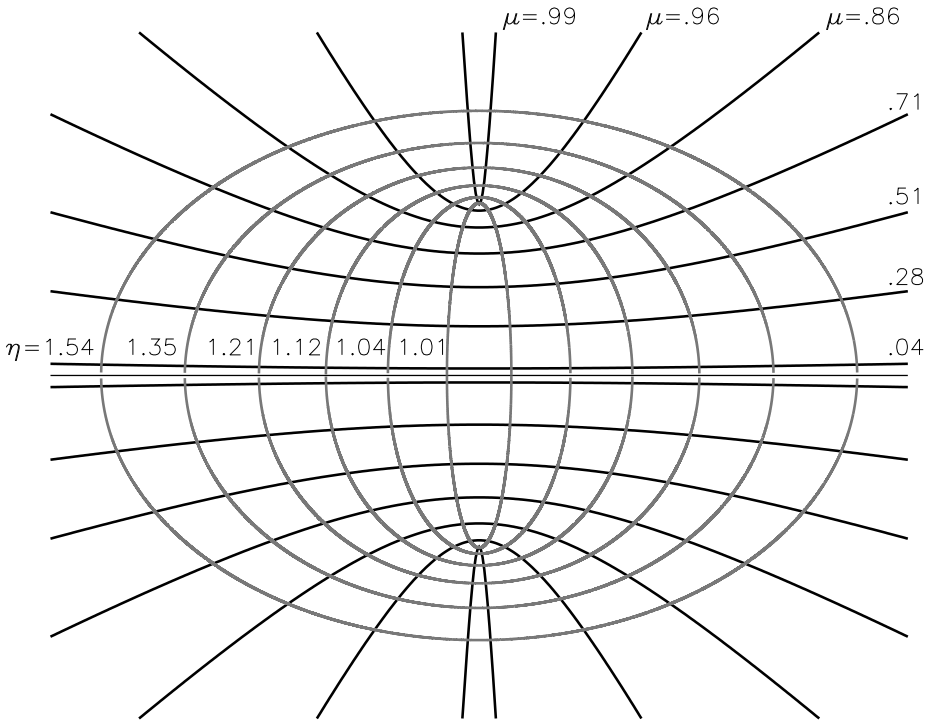

FIG. 6: Prolate Spheroidal Coordinate System. The projection of the confocal hyperboloids of revolution and the corresponding orthogonal spheroids of revolution onto the $\varphi = 0$ plane, where φ is the azimuthal coordinate. An arbitrary point in this system is identified with $\bar{r} = (\eta, \mu, \varphi)$. The surface of a particular hyperboloid is represented by fixing $\mu = \cos\theta$ where θ is the angle between the asymptote to the hyperbolid and z axis, while fixing $\eta = \cosh\zeta$ represents the surface of a particular spheroid of revolution with η being related to the radial distance.

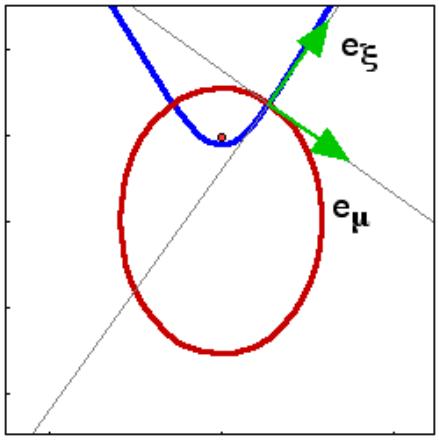

FIG. 7: Unit vectors of the modeling coordinate system, see (A10), and the special values (A11).

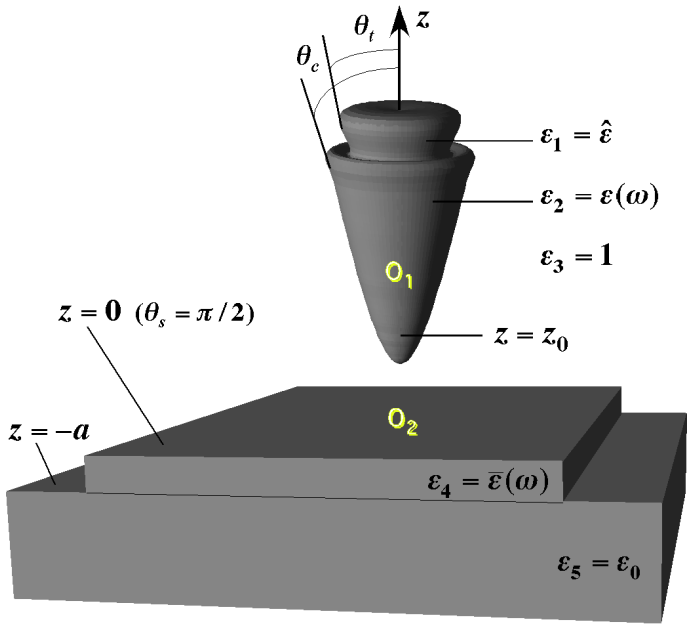

FIG. 8: Two truncated confocal hyperboloids represent the physical system of a coated probe $\mathbf{O_1}$. A third confocal hyperboloid defines the surface of the second object $\mathbf{O_2}$ to be probed. The $\epsilon_i, i = 1-5$ characterize the media involved.

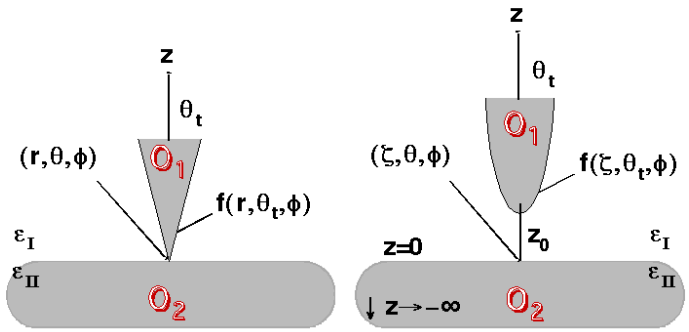

FIG. 9: The conical boundary can be used as a limiting case for a hyperboloid. Here ϵ_I defines the electrodynamic nature of the environment, while ϵ_{II} characterizes that of the material (shaded) domain.