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Operational WKB solution to the initial/final-value problem for Beechem-Haas equations *

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Abstract

Operational and Wantzel-Kramers-Brillouin (WKB) methods are utilized to obtain an analytical approximate solution of the Beechem-Haas equation for the initial/final-value problem with system parameters of radial profile. The Beechem-Haas equation herein is expanded from its traditional form, which determines its solutions in a spherical coordinate system as functions of the radial and time coordinates only, to one which includes the angular coordinates as well, thus providing a natural modeling framework for polarization phenomena.

1 Introduction

Consider the Beechem-Haas equation and its initial/boundary conditions, as given in [1],

$$\begin{gathered}\partial_t\overline{N}(r,t) = \Big(\textstyle\sum_{j=1}^{n} \frac{\alpha_j}{\tau_j}(1+(R_0/r)^6)\Big)\overline{N}(r,t) + \frac{1}{N_0(r)}\partial_r[N_0(r)D(r)\partial_r\overline{N}(r,t)]\,,\\ \overline{N}(r,t)\Big|_{t=0} = 1\,, \quad \overline{N}_{t=0}(r,t) = 1\,, \\ \partial_r\overline{N}(r,t)\Big|_{r=r_{\min}} = 0\,, \quad \partial_r\overline{N}(r,t)\Big|_{r=r_{\max}} = 0\,,\end{gathered} \tag{1}$$

where $0 < r_{\min} \le r \le r_{\max}$, $t \ge 0$, and α_j, τ_j, R_0 are positive real numbers. Unless otherwise directed, all variables, parameters, and domains are real.

In the present work, the full 3-dimensional form of the spatial derivatives in spherical coordinates shall be applied to (1), resulting in an enhanced form of the Beechem Haas equation, which will allow for the inclusion of angular components to the solution in a natural way. Particularly, this allows (1) to be

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extended to include the nontrivial effect of angular coupling to the radial component of the density function (i.e., polarization phenomena). Finally, the solution of the initial/final-value problem for the enhanced version of the Beechem-Haas equation will be addressed herein. This is basically the "on/off" control problem in the time-domain for the system. As a result of solving this problem, one then determines the system function necessary to produce a required output state, given a prescribed input state. Full technical details of the terms in (1), other than those supplied herein, are unnecessary for the present work. Therefore, the interested reader is encouraged to examine the original source [1]. The primary purpose of the present work is to simply supply a derivation of the results named above; applications and deeper studies shall appear elsewhere.

2 Main result

With these notions in place, the enhanced Beechem-Haas equation equation with attendant generalized auxiliary conditions becomes

$$\begin{aligned} \partial_t \overline{N}_E(r,\theta,\phi,t) &= \Big(\textstyle\sum_{j=1}^n \frac{\alpha_j}{\tau_j}(1+(R_0/r)^6)\Big)\overline{N}_E(r,\theta,\phi,t) \\ &\quad + \tfrac{4\pi r^2}{N_0(r)}\nabla\cdot[\tfrac{N_0(r)}{4\pi r^2}D(r)\nabla\overline{N}_E(r,\theta,\phi,t)]\,, \qquad (2) \\ \overline{N}_E(r,\theta,\phi,t)\Big|_{t=0} &= \overline{N}_{E_{t=0}}(r)\,, \quad \overline{N}_E(r,\theta,\phi,t)\Big|_{t=T} = \overline{N}_{E_{t=T}}(r) \\ \partial_r[\overline{N}_E(r,\theta,\phi,t)\Big|_{r=r_{\min}} &= 0\,, \quad \partial_r[\overline{N}_E(r,\theta,\phi,t)\Big|_{r=r_{\max}} = 0\,, \end{aligned}$$

where $0 < r_{\min} \le r \le r_{\max}$, $0 \le \theta \le \pi$, $0 \le \phi \le 2\pi$, $t \ge 0$, and α_j, τ_j, R_0 are positive real numbers. Expanding the above expression,

$$\begin{aligned} &\frac{1}{D(r)}\partial_t\overline{N}_E(r,\theta,\phi,t) \\ &= \frac{1}{D(r)}\Big(\sum_{j=1}^n \frac{\alpha_j}{\tau_j}(1+(R_0/r)^6)\Big)\overline{N}_E(r,\theta,\phi,t) \qquad (3) \\ &\quad +\nabla[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]\cdot\nabla\overline{N}_E(r,\theta,\phi,t) + \Delta\overline{N}_E(r,\theta,\phi,t)\,. \end{aligned}$$

Recall that the finite Fourier transform and its inverse [2] are defined as

$$\widehat{f}(n) = F_T[f(t)] = \int_0^T f(t)e^{-in\omega t}\,dt\,,$$

$$f(t) = F_T^{-1}[\widehat{f}(n)] = \frac{1}{T}\big(\widehat{f}(0) + \sum_{n=1}^{\infty}[\widehat{f}(n)e^{in\omega t} + \widehat{f}(-n)e^{-in\omega t}]\big)$$

Applying the finite Fourier transform on the time domain of (3), we obtain

$$\frac{1}{D(r)}[\overline{N}_{E_{t=T}}(r) - \overline{N}_{E_{t=0}}(r)]$$

$$\begin{aligned} &= \frac{1}{D(r)}\left(\sum_{j=1}^{n}\frac{\alpha_j}{\tau_j}(1+(R_0/r)^6)-in\omega\right)\widehat{N}_E(r,\theta,\phi,n) \qquad (4)\\ &\quad +\nabla[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]\cdot\nabla\widehat{N}_E(r,\theta,\phi,n)+\Delta\widehat{N}_E(r,\theta,\phi,n)\,. \end{aligned}$$

Reducing this to canonical form,

$$\begin{aligned} &\frac{1}{D(r)}[\overline{N}_{E_{t=T}}(r)-\overline{N}_{E_{t=0}}(r)]\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\\ &= \Delta\widetilde{N}_E(r,\theta,\phi,n)+\left(\frac{1}{D(r)}\big(\sum_{j=1}^{n}\frac{\alpha_j}{\tau_j}(1+(R_0/r)^6)-in\omega\big)\right. \qquad (5)\\ &\quad \left.-\frac{1}{2}\Delta[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]-\frac{1}{4}\left|\nabla[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]\right|^2\right)\widetilde{N}_E(r,\theta,\phi,n)\,, \end{aligned}$$

where

$$\begin{aligned} &\widetilde{N}_E(r,\theta,\phi,n)=\widehat{N}_E(r,\theta,\phi,n)\sqrt{\frac{N_0(r)D(r)}{4\pi r^2}}\,,\\ &\partial_r[\widetilde{N}_E(r,\theta,\phi,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}]\Big|_{r=r_{\min}}=0\,,\\ &\partial_r[\widetilde{N}_E(r,\theta,\phi,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}]\Big|_{r=r_{\max}}=0\,. \end{aligned}$$

Now we consider the homogeneous equation corresponding to (5),

$$\begin{aligned} 0 &= \Delta\widetilde{N}_{E_h}(r,\theta,\phi,n)+\left(\frac{1}{D(r)}\big(\sum_{j=1}^{n}\frac{\alpha_j}{\tau_j}(1+(R_0/r)^6)-in\omega\big)\right. \qquad (6)\\ &\quad \left.-\frac{1}{2}\Delta[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]-\frac{1}{4}\left|\nabla[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]\right|^2\right)\widetilde{N}_{E_h}(r,\theta,\phi,n)\,. \end{aligned}$$

Let $\widetilde{N}_{E_h}(r,\theta,\phi,n)=R_c(r,n)\Theta(\theta)\Phi(\phi)$. Then via separation of variables,

$$\begin{aligned} &\frac{1}{r^2R_c(r,n)}D_r(r^2D_rR_c(r,n))\\ &+\frac{1}{r^2\sin(\theta)\Theta(\theta)}D_\theta(\sin(\theta)D_\theta\Theta(\theta))+\frac{1}{r^2\sin^2(\theta)\Phi(\theta)}D_\theta^2\Phi(\theta) \qquad (7)\\ &= \frac{1}{D(r)}\big(\sum_{j=1}^{n}\frac{\alpha_j}{\tau_j}(1+(R_0/r)^6)-in\omega\big)\\ &\quad -\frac{1}{2}\Delta[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]-\frac{1}{4}\left|\nabla[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]\right|^2. \end{aligned}$$

Hence

$$D_r^2(rR_c(r,n)) - \Big(\frac{\lambda}{r^2} + \frac{1}{D(r)}\big(\sum_{j=1}^{n}\frac{\alpha_j}{\tau_j}(1+(R_0/r)^6) - in\omega\big) \qquad (8)$$

$$-\frac{1}{2}\Delta[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)] - \frac{1}{4}\Big|\nabla[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]\Big|^2\Big) rR_c(r,n) \quad = \quad 0\,,$$

$$\frac{1}{\Phi(\phi)}D_\phi^2\Phi(\phi) = -m^2\,,$$

$$\frac{1}{\sin\theta}D_\theta(\sin(\theta)D_\theta\Theta(\theta)) - \frac{m^2}{\sin^2\theta}\Theta(\theta) + \lambda\Theta(\theta) = 0\,,$$

where herein λ, m are arbitrary real parameters and n is a positive integer.

Regarding the solutions of the above angular component equations, they are most generally expressed as

$$\begin{aligned}\Theta(\theta)\Phi(\phi) \quad = \quad & [c_{\phi_1}e^{im\phi} + c_{\phi_2}e^{-im\phi}] \qquad (9)\\ & \times\Big(c_{\theta_1}\frac{1}{\Gamma(1-m)}\big(\frac{1+\cos\theta}{1-\cos\theta}\big)^{m/2} + c_{\theta_2}\frac{\pi\cot(m\pi)}{2\Gamma(1-m)}\big(\frac{1+\cos\theta}{1-\cos\theta}\big)^{m/2}\\ & -c_{\theta_2}\frac{\pi\Gamma(m+\lambda+1)}{2\sin(m\pi)\Gamma(\lambda-m+1)\Gamma(1+m)}\big(\frac{1+\cos\theta}{1-\cos\theta}\big)^{-m/2}\Big)\\ & \times F_{2,1}(-\lambda,\lambda;1-m;\frac{1-\cos\theta}{2})\,,\end{aligned}$$

where c_{ϕ_1}, c_{ϕ_2}, c_{θ_1}, c_{θ_2} are arbitrary constants. From (8) it is clear that the radial ordinary differential equation couples to the angular ordinary differential equation only when λ is non-zero. When $\lambda \neq 0$, (9) can take different forms, depending on the values of λ and m, which may be arbitrary real numbers. Indeed for λ and m integers, the angular dependence may be specified in terms of a finite superposition of spherical harmonics $Y_\lambda^m(\theta,\phi)$, rather than via the Gauss hyper-geometric functions $F_{2,1}$ used in in (9).

However, even if m is an integer and λ is not so restricted, the angular solutions will still [in general, by necessity] require the Gauss hyper-geometric formulation [3]. With an eye toward future results, the phenomena modeled by (8) may or may not require λ and m to be integer, depending upon the possible presence of more general non-homogeneous auxiliary conditions. For economy of notation result (9) may be denoted as $\Lambda(\theta,\lambda:\phi,m)$ in general. However, since the present homogeneous auxiliary conditions on the solutions are just the standard ones for boundedness and single-valuedness, it is here sufficient to particularly designate the angular components as spherical harmonics $Y_\lambda^m(\theta,\phi)$ with λ and m integers. Hence

$$\widetilde{N}_{Eh}(r,\theta,\phi,n) = R_c(r,n)\Theta(\theta)\Phi(\phi) = R_c(r,n)\Lambda(\theta,\lambda:\phi,m) = R_c(r,n)Y_\lambda^m(\theta,\phi)\,. \qquad (10)$$

The bulk of the remaining analysis concerns the radial equation (8). Now applying the WKB admissibility criterion [4] to (8),

$$\begin{aligned}\Phi(r,n) &= -\frac{\lambda}{r^2} - \frac{1}{D(r)}\big(\sum_{j=1}^{n}\frac{\alpha_j}{\tau_j}(1+(R_0/r)^6) - in\omega\big) \qquad (11)\\ &\quad +\frac{1}{2}\Delta[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)] + \frac{1}{4}\Big|\nabla[\ln\big(\frac{N_0(r)D(r)}{4\pi r^2}\big)]\Big|^2,\\ &\quad \frac{|D_r\Phi(r,n)/2|}{|\Phi(r,n)|^{3/2}} \ll 1\,.\end{aligned}$$

Hence the WKB results are accurate when the above criterion is met by the coefficient over the given (r,n)-domain. Recalling (10), there obtains the linearly independent WKB analytical solutions for the homogeneous radial equation in (8):

$$\begin{aligned}R_{c_1}(r,n) &\approx R_{c_1\mathrm{WKB}}(r,n)\\ &= \begin{cases}(-\Phi(r,n))^{-1/4}\cos(\int(-\Phi(r,n))^{1/2}\,dr) & \text{if } \Phi(r,n)<0,\\ (\Phi(r,n))^{-1/4}\exp(\int(\Phi(r,n))^{1/2}\,dr) & \text{if } 0<\Phi(r,n).\end{cases}\\ R_{c_2}(r,n) &\approx R_{c_2\mathrm{WKB}}(r,n) \qquad (12)\\ &= \begin{cases}(-\Phi(r,n))^{-1/4}\sin(\int(-\Phi(r,n))^{1/2}\,dr) & \text{if } \Phi(r,n)<0,\\ (\Phi(r,n))^{-1/4}\exp(-\int(\Phi(r,n))^{1/2}\,dr) & \text{if } 0<\Phi(r,n).\end{cases}\end{aligned}$$

Hence, the general solution of the radial part of the full non-homogeneous equation (5) may be supplied via (12) as

$$\begin{aligned}&c_1(n)R_{c_1}(r,n) + c_2(n)R_{c_2}(r,n) \qquad (13)\\ &+R_{c_2}(r,n)\int\frac{\overline{N}_{E_{t=T}}(r) - \overline{N}_{E_{t=0}}(r)}{D(r)\widetilde{w}(r,n)}R_{c_1}(r,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\,dr\\ &-R_{c_1}(r,n)\int\frac{\overline{N}_{E_{t=T}}(r) - \overline{N}_{E_{t=0}}(r)}{D(r)\widetilde{w}(r,n)}R_{c_2}(r,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\,dr\,,\end{aligned}$$

where

$$\widetilde{w}(r,n) = R_{c_1}(r,n)D_rR_{c_2}(r,n) - R_{c_2}(r,n)D_rR_{c_1}(r,n)\,.$$

By ansatz (10), (13), and (5), the time-transformed version (4) of equation (12) has general solution

$$\begin{aligned}\widehat{N}_E(r,\theta,\phi,n) &= \sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\widetilde{N}_E(r,\theta,\phi,n)\\ &= \sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}Y_\lambda^m(\theta\phi)\Big(c_1(n)R_{c_1}(r,n) + c_2(n)R_{c_2}(r,n) \qquad (14)\\ &\quad +R_{c_2}(r,n)\int\frac{\overline{N}_{E_{t=T}}(r) - \overline{N}_{E_{t=0}}(r)}{D(r)\widetilde{w}(r,n)}R_{c_1}(r,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\,dr\end{aligned}$$

$$-R_{c_1}(r,n)\int \frac{\overline{N}_{E_{t=T}}(r)-\overline{N}_{E_{t=0}}(r)}{D(r)\widetilde{w}(r,n)} R_{c_2}(r,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\,dr\Bigg)\,,$$

Now consider the boundary conditions of (4), which are the time-transformed boundary conditions of (1),

$$\partial_r \widehat{N}_E(r,\theta,\phi,n)\Big|_{r=r_{\rm min}} = 0\,,\quad \partial_r \widehat{N}_E(r,\theta,\phi,n)\Big|_{r=r_{\rm max}} = 0\,. \tag{15}$$

Without loss of generality, we may ignore the angular factor $Y_\lambda^m(\theta\phi)$ and consider only the radial terms in (14). Given the particular boundary conditions (15), the formula (14) may be used to calculate the appropriate particular solution matching the boundary conditions in the (r,n)-domain. In general, there will result a 2x2 matrix equation for the coefficients $c_1(n)$ and $c_2(n)$.

$$\begin{pmatrix} P_{11} & P_{21} \\ P_{21} & P_{22} \end{pmatrix} \begin{pmatrix} c_1(n) \\ c_2(n) \end{pmatrix} = \begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix}\,, \tag{16}$$

where

$$P_{11} = \partial_t\Bigg(\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}R_{c_1}(r,n)\Bigg)\Bigg|_{r=r_{\rm min}}\,,$$

$$P_{12} = \partial_t\Bigg(\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}R_{c_2}(r,n)\Bigg)\Bigg|_{r=r_{\rm min}}\,,$$

$$P_{21} = \partial_t\Bigg(\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}R_{c_1}(r,n)\Bigg)\Bigg|_{r=r_{\rm max}}\,,$$

$$P_{22} = \partial_t\Bigg(\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}R_{c_2}(r,n)\Bigg)\Bigg|_{r=r_{\rm max}}\,,$$

$$Q_1 = -\partial_r\Bigg(R_{c_2}(r,n)\int \frac{\overline{N}_{E_{t=T}}(r)-\overline{N}_{E_{t=0}}(r)}{D(r)\widetilde{w}(r,n)} R_{c_1}(r,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\,dr$$

$$-R_{c_1}(r,n)\int \frac{\overline{N}_{E_{t=T}}(r)-\overline{N}_{E_{t=0}}(r)}{D(r)\widetilde{w}(r,n)} R_{c_2}(r,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\,dr\Bigg)\Bigg|_{r=r_{\rm min}}\,,$$

$$Q_2 = -\partial_r\Bigg(R_{c_2}(r,n)\int \frac{\overline{N}_{E_{t=T}}(r)-\overline{N}_{E_{t=0}}(r)}{D(r)\widetilde{w}(r,n)} R_{c_1}(r,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\,dr$$

$$-R_{c_1}(r,n)\int \frac{\overline{N}_{E_{t=T}}(r)-\overline{N}_{E_{t=0}}(r)}{D(r)\widetilde{w}(r,n)} R_{c_2}(r,n)\sqrt{\frac{4\pi r^2}{N_0(r)D(r)}}\,dr\Bigg)\Bigg|_{r=r_{\rm max}}\,.$$

Then by Cramer's Rule, the functions $c_1(n)$ and $c_1(n)$ have values

$$c_1(n) = \frac{P_{22}Q_1 - P_{21}Q_2}{P_{11}P_{22}-P_{21}P_{12}}\,,\quad c_2(n) = \frac{P_{11}Q_2 - P_{12}Q_1}{P_{11}P_{22}-P_{21}P_{12}}\,. \tag{17}$$

Hence the cefficients in (17) are the functions of n necessary for the given time-transformed boundary conditions of (15) to be met in (14). Finally, substituting the coefficients in (17) into (14), and applying the inverse finite Fourier transform to $\widehat{N}_E$ in (14) yields the operational WKB analytical solution to the boundary and initial/final value problem (2) in the (r,θ,ϕ,t)-domain.

$$\begin{aligned}\overline{N}_E(r,\theta,\phi,t) &= F_T^{-1}[\widehat{N}_E(r,\theta,\phi,n)] \\ &= \frac{1}{T}\big(\widehat{N}_E(r,\theta,\phi,0)+\sum_{n=1}^{\infty}[\widehat{N}_E(r,\theta,\phi,n)e^{in\omega t}+\widehat{N}_E(r,\theta,\phi,-n)e^{-in\omega t}]\big)\,,\end{aligned}$$

with $\widehat{N}_E(r,\theta,\phi,n)$ given by (14).

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