Reply to "On the Factorized Kernel Approach for Solving Multidimensional Neutron Transport Problems"

The letter by Sahni[1] offers me the possibility of clarifying some basic points in my recent paper.[2]

Contrary to what is affirmed by Sahni,[1] the equation

$$\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^2} = \frac{1}{2\pi^{3/2}}\int_0^\infty du\ \mathrm{erfc}(\Sigma u)\int_{(\infty)} d\boldsymbol{k}' \times \exp[-k'^2u^2 - i\boldsymbol{k}'\cdot(\boldsymbol{r}-\boldsymbol{r}')] \ , \tag{1}$$

can be generalized to the case of a kernel

$$F_n(|\boldsymbol{r}-\boldsymbol{r}'|) = \frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^n} \ , \qquad n \geqslant 2 \ , \tag{2}$$

in a completely correct and rigorous way.

The procedure (not explicitly presented in Ref. 2) we can follow in order to attain the generalization mentioned above does not at all imply a Fourier transformation of the function F_n generating the kernel in Eq. (2), contrary to what seems to be thought by Sahni.

In fact, we can first apply the simple result

$$\frac{\exp(-\alpha x)}{x^n} = \int_\alpha^\infty ds_1 \int_{s_1}^\infty ds_2 \ldots \int_{s_{n-3}}^\infty ds_{n-2} \frac{\exp(-s_{n-2}x)}{x^2} \ , \qquad n \geqslant 2 \ , \tag{3}$$

where $s_0 = \alpha \geqslant 0$ and no integrals appear for $n = 2$, to the right side of Eq. (2), and obtain

$$\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^n} = \int_\Sigma^\infty ds_1 \int_{s_1}^\infty ds_2 \ldots \int_{s_{n-3}}^\infty ds_{n-2} \frac{\exp(-s_{n-2}|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^2} \ , \qquad n \geqslant 2 \ , \tag{4}$$

with the same convention as before. Then let us take Eq. (1) into account, and write

$$\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^n} = \frac{1}{2\pi^{3/2}}\int_\Sigma^\infty ds_1 \int_{s_1}^\infty ds_2 \ldots \int_{s_{n-3}}^\infty ds_{n-2} \times \int_0^\infty du\ \mathrm{erfc}(s_{n-2}u) \times \int_{(\infty)} d\boldsymbol{k} \exp[-k^2u^2 - i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')] \ . \tag{5}$$

Thus, the unique Fourier transformation used until now is exactly that already considered in Sahni's paper.[3] The inverse Fourier transform, which constitutes the most internal integral in Eq. (5), can be performed to obtain the more explicit factorization

$$\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^n} = \frac{1}{2}\int_\Sigma^\infty ds_1 \int_{s_1}^\infty ds_2 \ldots \int_{s_{n-3}}^\infty ds_{n-2} \times \int_0^\infty du\ \mathrm{erfc}(s_{n-2}u)\frac{1}{u^3}\prod_{j=1}^3 \exp\left[-\left(\frac{r_j - r_j'}{2u}\right)^2\right] . \tag{6}$$

At this point Fubini's theorem for positive measurable functions allows inverting the order of the two last integrals over s_{n-2} and u, thus obtaining

$$\begin{aligned}\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^n} &= \frac{1}{2}\int_\Sigma^\infty ds_1 \int_{s_1}^\infty ds_2 \ldots \int_{s_{n-4}}^\infty ds_{n-3} \int_0^\infty du \frac{1}{u^3} \times \prod_{j=1}^3 \exp\left[-\left(\frac{r_j - r_j'}{2u}\right)^2\right] \cdot \int_{s_{n-3}}^\infty ds_{n-2}\,\mathrm{erfc}(s_{n-2}u) \\ &= \frac{1}{2}\int_\Sigma^\infty ds_1 \int_{s_1}^\infty ds_2 \ldots \int_{s_{n-4}}^\infty ds_{n-3} \int_0^\infty du \frac{1}{u^4} \times \prod_{j=1}^3 \exp\left[-\left(\frac{r_j - r_j'}{2u}\right)^2\right] i^1\,\mathrm{erfc}(s_{n-3}u) \ .\end{aligned} \tag{7}$$

When $n = 3$, the final result is directly reached, since integrals previous to that over u do not exist in Eq. (7). For $n > 3$, since the iterated integrals

$$i^k\,\mathrm{erfc}(x) = \int_x^\infty ds_1 \int_{s_1}^\infty ds_2 \ldots \int_{s_{k-1}}^\infty ds_k\,\mathrm{erfc}(s_k) \ ,$$

on the complementary error function

$$\mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty \exp(-t^2)dt \ ,$$

are in turn positive measurable functions, an iterative application of Fubini's theorem gives our final result in the form

$$\frac{\exp(-\Sigma|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^n} = \frac{1}{2}\int_0^\infty du \frac{i^{n-2}\,\mathrm{erfc}(\Sigma u)}{u^{n+1}}\prod_{j=1}^3 \exp\left[-\left(\frac{r_j - r_j'}{2u}\right)^2\right] . \tag{8}$$

Let us remark that the integral representation at the right side of Eq. (8) exhibits, as expected, the same singular behavior of the left side. In fact, let us rewrite the product in Eq. (8) as

$$\prod_{j=1}^3 \exp\left[-\left(\frac{r_j - r_j'}{2u}\right)^2\right] = \exp\left[-\frac{|\boldsymbol{r}-\boldsymbol{r}'|^2}{4u^2}\right] ,$$

according to Ref. 1, and make the change of variable $x = u/|\boldsymbol{r}-\boldsymbol{r}'|$. Then the right side of Eq. (8) becomes

$$\frac{1}{2}\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|^n}\int_0^\infty dx \frac{i^{n-2}\,\mathrm{erfc}(\Sigma|\boldsymbol{r}-\boldsymbol{r}'|x)}{x^{n+1}}\exp\left[-\frac{1}{(2x)^2}\right] . \tag{9}$$

The integral in Eq. (9) is clearly convergent to a positive value for any $|\boldsymbol{r}-\boldsymbol{r}'|$ and goes to 2 for $|\boldsymbol{r}-\boldsymbol{r}'| \to 0$. Once it is established that Eq. (8) is valid, we can see that our approach allows the treatment of scattering anisotropy of arbitrary order, while the treatment proposed by Sahni[1] considered, up to now, linearly anisotropic scattering only, as far as I know.

Further, the algorithms for the computation of matrix elements developed in Ref. 2 represent a very useful and significant contribution, as recognized in Ref. 1. The efficiency of such algorithms stresses again the usefulness of our approach.

Of course we appreciated very much Sahni's previous works in this field, especially Ref. 3, already quoted in Ref. 2, which opened a wide field to applications and research and constituted a fundamental reference for us, both from a theoretical and a numerical point of view. Matrix elements involved in the Fourier transform method developed originally in Ref. 4 for three-dimensional parallelepiped, once factorized

[1] D. C. SAHNI, *Nucl. Sci. Eng.*, **74**, 65 (1980).

[2] A. BASSINI, F. PREMUDA, and W. A. WASSEF, *Nucl. Sci. Eng.*, **71**, 87 (1979).

[3] D. C. SAHNI, *J. Nucl. Energy*, **26**, 367 (1972).

[4] V. C. BOFFI and V. G. MOLINARI, *Trans. Th. Stat. Phys.*, **1**, 313 (1971).

in Ref. 3, became computable as did rectangular geometry and finite cylinder matrix elements, so opening to the specific Fourier transform method the actual possibility of very accurate multidimensional numerical applications. On the other hand, from a theoretical point of view Sahni's idea constituted the starting point for the foundation of a much more widely applicable approach. Actually, once the generalization to $n > 2$ of the Sahni formula [Eq. (1)] was reached by Eq. (5), the natural transition to Eqs. (6) and (8) allowed reaching a true factorization of the kernels of the integral transport formulation in the original Euclidean space, so leaving completely free the choice of the method to be adopted in subsequently solving the problem, when the choice was previously restricted to the unique Fourier transform method.

In Ref. 2, once the kernels were factorized, a decomposition of the kernel into Legendre polynomials (DKPL) method of solution was chosen and polynomial and iterated fluxes were obtained by avoiding the introduction of Fourier transformed equations, Bessel functions, and inverse Fourier transform. Though methods based on Fourier transform repeatedly used by the neutron physics group of Bologna[5-12] have shown their heuristic power in Ref. 3, and this will surely happen again in the future, we must recognize that the restriction removed in factorizing the kernels directly in the original Euclidean space is far from being useless; in fact, the treatment of heterogeneous multidimensional geometries by the Fourier transform method encounters difficulties, whereas a new method based on integral transport equation proposed by Stepanek[13] and new formulations[14,15] of the integral transport DKPL method are able to treat such problems by decoupling different regions and representing the effects of the whole system on a single region by pure interface interactions.

Finally the possibility of applying different methods, with respect to DKPL, to the integral transport equation with factorized kernels already had at least one application in a work applying the modal-nodal tensorial diffusion approach to the integral transport equation in parallelepiped geometry[16] giving rise to a new computational program.[17]

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