Computer Code Abstract

TISK

A Program for Calculating Thermal Neutron Scattering Kernels

1. Name of Program: TISK
2. Computer for Which Program is Designed: UNIVAC-1108.
3. Nature of Problem Solved: The code computes either the thermal neutron scattering law $S(\alpha, \beta)$, or the zeroth and first Legendre moments $[\sigma_0(E_0 \rightarrow E), \sigma_1(E_0 \rightarrow E)]$ of the scattering cross section.
4. Method of Solution: The Egelstaff-Schofield representation of $S(\alpha, \beta)$ as a cosine transform is used. For the angular moments, this representation is integrated analytically over the angular variable to obtain representations of σ_0 and σ_1 themselves as cosine transforms. In either case, the transforms are evaluated by integrating over successive half-cycles of the cosine using Simpson's rule, and then summing the resulting alternating series using an Euler transform to minimize accrual of round-off error. When appropriate, the contributions to the integral from large values of t are evaluated from analytical expressions, with only the contributions from smaller t values being computed numerically. For large momentum-transfers and large E_0, asymptotic expansions of $S(\alpha, \beta)$ and the $\sigma_n(E_0 \rightarrow E)$ are used instead. TISK performs these computations with any user-supplied function routine for the width function $w(t)$. However, a versatile width generator is supplied with the code, and is based on a representation of the spectral function $\rho(\beta)$ as a sum of resonance-like peaks containing many adjustable parameters. In particular, a set of parameters for room temperature light water is available.
5. Restrictions on the Complexity of the Problem: As presently programmed, the number of energy groups must not exceed 101. Neither the number of α-values, nor the number of β-values may exceed 100.
6. Typical Running Time: Highly dependent on the complexity of the spectral function $\rho(\beta)$.
7. Unusual Features of the Program: Either energy groups, or energy points may be specified routinely. For the elastic case $(E = E_0)$, the average of the $\sigma_n(E_0 \rightarrow E)$ over a narrow elastic group is computed directly, since the values at the point $E = E_0$ may be infinite. It is possible to evaluate the $\sigma_n(E_0 \rightarrow E)$ for a subset of the desired energy set, and to restart a run aborted for lack of time without loss of previously computed information.
8. Related and Auxilliary Programs: None.
9. Status; TISK is in use on the UNIVAC 1108 computer, Computer Sciences Corporation, Richland, Washington.
10. Machine Requirements: 64K memory, normal input, output, program and punch units.
11. Programming Language Used: All routines are written in FORTRAN-V, except for a rounding routine written in assembly language.
12. Operating System or Monitor under Which Programs are Executed: UNIVAC 1108 Computer with FORTRAN-V compiler and CSCX operating system.
13. Other Programming or Operating Information or Restrictions: Program TISK has 33 subroutines and ~1500 source cards.
14. Material Available: The codes and documentation may be obtained through the Argonne Code Center, Argonne National Laboratory.
15. Acknowledgment: This work was funded by the U.S. Atomic Energy Commission contract AT(45-1)-1830.
16. *References*:

[1]A. G. GIBBS and C. W. LINDENMEIER, "TISK, a Program for Calculating Thermal Neutron Scattering Kernels, and its Application to H_2O," BNWL-1675, Battelle, Pacific Northwest Laboratories (1972).

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