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Schwinger Variational Principle for Multichannel Scattering

Kazuo Takatsuka and Vincent McKoy
Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125
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This Letter presents the first application of the Schwinger variational principle for multichannel scattering. Results are presented for an exactly soluble two-channel model problem. The accuracy and convergence of the Schwinger variational principle are shown to be extremely good and superior to those of other variational methods.

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In spite of several desirable features, the Schwinger variational principle[1,2] has not been applied extensively to scattering problems. Several recent applications[3-7] of the Schwinger principle to single-channel electron-molecule collision problems demonstrated the potential of the Schwinger method. Furthermore, we are currently extending the Schwinger method to multichannel problems on the basis of a new formulation. In order to assess the effectiveness and accuracy of the Schwinger method for multichannel cases, we have solved the model two-channel problem proposed by Huck[8] prior to its application to actual systems. In this application, we have found that the Schwinger method is extremely effective yielding results far more striking than those of sophisticated versions of the standard variational principles.[9-12] As far as we know, this is the first example of the application of the Schwinger principle to a multichannel problem.

The exactly soluble two-channel model problem used by Huck,[8] Nesbet,[9-11] and more recently by Harris,[12] is defined by the Hamiltonian $H = H_0 + V$ with

$$H_0 = |\chi_1\rangle(-\tfrac{1}{2}d^2/dr^2)\langle\chi_1| + |\chi_2\rangle[-\tfrac{1}{2}d^2/dr^2 + \Delta E]\langle\chi_2| , \quad (1)$$

and

$$V = \sum_{m\neq n}^{2} |\chi_m\rangle V_{mn}\langle\chi_n| , \quad (2)$$

where

$$V_{12} = V_{21} = \begin{cases} \tfrac{1}{2}C, & r < a \\ 0, & r > a, \end{cases} \quad (3)$$

and $\langle\chi_m|\chi_n\rangle = \delta_{mn}$. In terms of the regular eigenfunctions of H_0,

$$S_m(r_1, r_2) = \chi_m(r_1) k_m^{-1/2} \sin k_m r_2, \quad m = 1, 2, \quad (4)$$

the variational functional for the K matrix is given by

$$[K_{mn}] = \frac{\langle\Psi_m|U|S_n\rangle\langle S_m|U|\Psi_n\rangle}{\langle\Psi_m|(UG_0U - U)|\Psi_n\rangle}, \quad (5)$$

where $U = 2V$. In Eq. (5), the free-particle (standing-wave) Green's function G_0 is

$$G_0(r_1, r_2; r_1' r_2') = -\sum_{m=1}^{2} S_m(r_1, r_<) C_m(r_1', r_>), \quad (6)$$

where C_m is the irregular solution of H_0, and $r_> = \max(r_2, r_2')$ and $r_< = \min(r_2, r_2')$. It should be noted that the above Green's function has a very simple structure, since no permutation symmetry is imposed on the wave functions Ψ_m $(m = 1, 2)$. As usual, the wave function is expanded in terms of a basis set $\{\eta_i^m | m = 1, 2; i = 1, \ldots, N\}$. From the stationary condition $\delta[K_{mn}] = 0$, the K-matrix elements can be written as

$$K_{mn} = \sum_{a,b}^{2} \sum_{i,j}^{N} \langle S_m|U|\eta_i^a\rangle D_{ij}^{ab} \langle\eta_j^b|U|S_n\rangle, \quad (7)$$

where

$$(D^{-1})_{ij}^{ab} = \langle\eta_i^a|(UG_0U - U)|\eta_j^b\rangle. \quad (8)$$

In order to compare with the previous results of Nesbet *et al.*[9-11] and Harris and Michels[12] and the exact results,[9] we also choose the potential parameters $a = 1.0$ and $C^2 = 10.0$, and the energies

$E = 0.5$, and $\Delta E = 0.375$ ($k_1 = 1.0$ and $k_2 = 0.5$). For our calculation, the basis set is composed of only the L^2 functions

$$\eta_i^m = |\chi_m\rangle r^i e^{-pr}, \quad i = 1, 2, \ldots, N, \tag{9}$$

since the total energy ($E = 0.5$) is sufficiently lower than the height of the potential ($\frac{1}{2}C \sim 1.58$). However, in the high-energy region where the Born approximation is valid, it would be necessary to include the long-range function in the basis. The optimum value of the parameter p for η_i^m was determined to be 2.5 by Nesbet[9] and Harris[12] for their variational methods.

The double integrals $\langle \eta_i^a | (UG_0U - U) | \eta_j^b \rangle$ appearing in Eq. (9) are evaluated using a 32-point Gaussian quadrature. The use of the recursion formula makes this double integration efficient and accurate. The general procedure for the integral UG_0U has already been described elsewhere[5] and also will be discussed in our later publication.

In Table I, we show the deviation (ΔK) of the K matrices obtained from the Schwinger variational principle from the exact results as a function of the basis set size N. The computational results in terms of two different basis sets with the exponent $p = 2.5$ (the same as that for the other methods) and 0.9 (optimized value for the Schwinger principle) are listed.

To compare and to emphasize the accuracy of the Schwinger method we also show the deviations of the K matrices obtained by Nesbet by means of the anomaly-free (AF),[9] optimized anomaly-free (OAF),[10] and restricted interpolated anomaly-free (RIAF)[11] methods and by Harris and Michels with the minimum-norm (MN)[12] method. Our results are quite clear and impressive. The rate of the convergence of the Schwinger method with $p = 2.5$ is much faster than those of the other methods. For instance, the Schwinger K matrix with two basis functions ($N = 2$) is already closer to the exact value than the K matrices of the other methods with use of 25 basis functions. Furthermore, with $N = 6$, the Schwinger K matrices

TABLE I. The deviation (ΔK) of the variationally determined K matrices from the exact values. The exact values are: $K_{11} = 21.765\,25$, $K_{12} = K_{21} = -14.127\,42$, and $K_{22} = 8.733\,85$ (see Ref. 9).

		AF[a]	MN[b]	OAF[c]	RIAF[d]	Schwinger ($p = 2.5$)[e]	Schwinger ($p = 0.9$)[e]
ΔK_{11}	N = 1	--	-18.72853	--	--	-19.09277	-0.14259
	2	--	-58.41920	--	--	- 0.26131	-1.53971
	4	-5.61743	- 5.69784	-4.54847	--	- 0.01000	-0.00004
	6	-2.99726	- 3.29061	-2.99989	-3.00448	0.0	0.0
	10	-1.39131	- 1.40472	-1.37881	-1.39040	0.0	0.0
	25	-0.36330	--	-0.33532	-0.29985	0.0	0.0
ΔK_{12}	N = 1	--	11.86603	--	--	12.10630	-0.09141
	2	--	37.84736	--	--	0.07861	0.96567
	4	3.57888	3.66193	2.89239	--	0.00600	0.00002
	6	1.91396	2.09620	1.91579	1.91839	0.0	0.0
	10	0.88909	0.89739	0.88115	0.88850	0.0	0.0
	25	0.23037	--	0.21363	0.19117	0.0	0.0
ΔK_{22}	N = 1	--	- 7.54469	--	--	- 7.57920	0.19492
	2	--	24.52584	--	--	0.01638	-0.60478
	4	-2.28298	- 2.35953	-1.84341	--	- 0.00355	-0.00002
	6	-1.22397	- 1.33719	-1.22525	-1.22670	0.0	0.0
	10	-0.56896	- 0.57410	-0.56393	-0.56858	0.0	0.0
	25	-0.14621	--	-0.13619	-0.12198	0.0	0.0

[a] Refs. 9 and 10.
[b] Ref. 12.
[c] Refs. 10 and 11.
[d] Ref. 11.
[e] The exponent in the basis functions.

have almost completely converged to the exact values, whereas the results of the other vibrational methods are still far from being converged. As can be seen from the table, the K matrix of the Schwinger principle with $N=1$ is worse than that of the MN method. This implies simply that the basis functions with $p=2.5$ are not the best for the Schwinger principle, even though they are the best for the standard variational principles.[12] In fact, the best K matrix of the Schwinger method with $N=1$ was found to be given for a value of 0.9 for the parameter p in Eq. (9). In this case, K_{11} and K_{12} $(=K_{21})$ of the Schwinger method are better than those of the other variational methods even with $N=25$. We have made this comparison between the Schwinger and Kohn-type methods only at one energy since the Kohn-type methods have not been applied to this model problem at any other energies. It would be interesting to extend the present comparison of these methods to other energies.

A comparison of the cross sections (Q_{mn}) is shown in Table II. The cross section is much less sensitive than the K matrix. The cross sections at $N=2$ are a good example: The minimum-norm method gives better cross sections than the Schwinger method with $p=2.5$ in spite of the fact that this method gave the worst K matrix at $N=2$. However, for N greater than 2, the Schwinger method gives the best results. With six basis functions, the cross sections from the Schwinger method coincide with the exact ones. The convergence is faster than const$\times 10^{-N}$ $(\Delta Q_{N+1}/\Delta Q_N < \text{const}\times 10^{-1})$ for almost all N. Again, more impressive results are obtained by means of the Schwinger principle using the basis functions of $p=0.9$. The deviations are roughly ten times smaller than those of the Schwinger method with

TABLE II. The deviation of the computed cross sections from the exact ones. The exact cross sections, $Q_{11}=2.167\,91$, $Q_{12}=0.767\,46$, $Q_{21}=3.069\,85$, and $Q_{22}=2.558\,44$. See Ref. 9. ΔQ_{mn} (in units of πa_0^2).

	N	AF[a]	MN[b]	Schwinger ($p=2.5$)[c]	Schwinger ($p=0.9$)[c]
ΔQ_{11}	1	-0.27129	-0.26426	-0.42134	-0.04145
	2	-0.01387	-0.01336	-0.02142	-0.00516
	3	-0.04953	-0.02550	-0.00173	-0.00049
	4	-0.00807	0.00068	-0.00009	0.0
	5	-0.00330	-0.00193	0.00000	0.0
ΔQ_{12}	1	0.08584	0.08055	0.10898	0.01342
	2	0.00517	-0.01268	0.00708	0.00215
	3	0.00665	0.01399	0.00058	0.00003
	4	0.00475	0.00200	0.00003	0.0
	5	0.00226	0.00200	0.00000	0.0
ΔQ_{21}	1	0.34334	0.32220	0.43591	0.05366
	2	0.02068	-0.05074	0.02832	0.00860
	3	0.02659	0.05596	0.00230	0.00011
	4	0.01899	0.00800	0.00013	0.0
	5	0.00903	0.00801	0.00000	0.0
ΔQ_{22}	1	0.00454	-0.12261	-0.55696	-0.04418
	2	0.03600	0.18866	-0.02922	-0.00262
	3	0.16017	-0.02510	-0.00146	-0.00005
	4	-0.00219	0.00304	-0.00007	-0.00001
	5	-0.00122	-0.00186	-0.00001	0.0

[a]Ref. 9.
[b]Ref. 12.
[c]The exponent in the basis functions.

$p = 2.5$.

As presented in this Letter, the Schwinger method for the multichannel scattering has been shown to yield much better results than those of other variational methods. The rapid convergence is dramatic. In conclusion, the Schwinger variational principle is quite promising and encouraging for the multichannel scattering as well as for the single-channel case.

Recently Thirumalai and Truhlar[13] carried out a series of calculations on an attractive exponential potential which were designed to compare the convergence of the Schwinger variational principle with that of the Kohn method. They concluded that the Kohn-type methods show much better convergence to the accurate result than the Schwinger method. Unfortunately the same trial scattering wave functions were not used in these two variational principles. We have repeated these calculations using the same trial wave functions in the Schwinger and Kohn variational principles and find that the Schwinger procedure gives superior results.[14] Hence these results are in fact consistent with the trend seen in the present application of these methods to this two-channel model problem. Details of these calculations and a discussion of the mathematical relationship between the Schwinger and Kohn variational methods will be published elsewhere.[14]

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Heating by Raman Backscatter and Forward Scatter

Kent Estabrook, W. L. Kruer, and B. F. Lasinski

Lawrence Livermore Laboratory, University of California, Livermore, California 94550

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This Letter presents computer simulations of the reflection and heating due to stimulated Raman scattering of intense laser light in large regions of underdense plasma. The heated electron distribution is approximately a Maxwellian of temperature $\frac{1}{2}m_e v_\phi^2$. A simple model of the reflection is presented. Forward Raman scattering was also observed producing extremely energetic electrons. Finally, two-dimensional simulations showed sizable Raman scattering coexisting with heating by the $2\omega_{pe}$ instability. Raman scattering may cause a preheat problem with large laser-fusion-reactor targets.

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Motivated by recent observations[1,2] of Raman scattering in reactor targets and the great interest in this process as a preheat source, we present computer simulations of the reflection and heating due to stimulated Raman backscattering of intense laser light in large regions of under-