(like τ') are estimated to be completely negligible at the statistical level of this experiment.

[14] One can also calculate the detection effeciency for $\pi^+\nu\bar{\nu}$ events from knowing that 217 $K_{\pi 2}$ events with no gammas pointing were detected. Assuming a reasonable gamma-ray detection efficiency one gets very good agreement with the conclusion that we would detect 10.6 % of a real sample of $\pi^+\nu\bar{\nu}$ events.

SYSTEMATIC CONSTRUCTION OF CORRELATED MANY-PARTICLE INTEGRAL-TRANSFORM TRIAL FUNCTIONS AND MULTICENTER MOLECULAR ORBITALS

R. L. Somorjai
Division of Pure Chemistry, National Research Council of Canada, Ottawa, Canada

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A systematic approach to the construction of new types of correlated many-particle trial functions is outlined. It is based on the formalism of a special type of multidimensional integral transformation, and combines a conceptually simple geometrical interpretation with computational practicability and the possibility of classifying the correlated wave functions in a simple manner. The approach is applicable to the formation of new, multicenter molecular orbitals as well.

Recently I proposed the use of integral-transform trial functions in quantum mechanical calculations.[1] Such functions are extremely efficient[2-5] and give rise to orbitals of near Hartree-Fock accuracy with only a few adjustable parameters. In this work we generalize and extend the idea in a systematic manner to correlated many-particle trial functions. The formalism is equally applicable for the construction of new kinds of molecular orbitals.

Let H be the Hamiltonian of the system whose solution $\varphi(x)$ we seek. Assume that the exact solution $\varphi_0(x)$ of some related model Hamiltonian H_0 is known. Then one constructs the integral-transform trial function $\varphi_1(x)$, an approximate solution to $\varphi(x)$, by formally scaling φ_0, $\varphi_0(x) \rightarrow \varphi_0(tx)$, and forming

$$\varphi_1(x) = \int_D S(t)\varphi_0(tx)dt, \tag{1}$$

where D is some suitable domain of integration and $S(t)$, called the shape function, is a weight factor to be determined. The computationally most practical approach is to parametrize some trial form of $S(t)$ and optimize the parameters variationally. The following simple argument[2] aids in the selection of an appropriate analytical form for $S(t)$: As the "perturbation" $(H-H_0)$ approaches zero, both $\varphi_0(tx)_{t=1}$ and $\varphi_1(x)$ tend to $\varphi(x)$. This is consistent only if in that limit $S(t) = \delta(t-1)$. Consequently one chooses a trial $S(t)$ which for certain limiting values of its parameters becomes the delta function, i.e., $S(t)$ should be a delta-convergent sequence.[6]

Since $\varphi_0(xt)$ is a function of the product xt, Mellin transform functions are the natural choice, as in the case of the iterated integral-transform-function approach[4] where the kth iteration $\varphi_k(x)$ is obtained by the prescription

$$\varphi_k(x) = \underbrace{\int \cdots \int}_{k\text{-fold}} \varphi_0(x \prod_{i=1}^{k} t_i) \prod_{i=1}^{k} S_i(t_i)dt_i.$$

One straightforward generalization[1] to many-particle systems is to take some relatively simple N-particle, M-parameter trial function of the independent-particle type and integrate it with respect to the parameters, choosing a suitable $S(t_1, t_2, \cdots, t_M)$. This involves an M-dimensional integration. Particle correlation is to be introduced by coupling the t_i in $S(\vec{t})$. One special version is to use the N scaling parameters as the integration variables t_i and again select some appropriate S. The main objection to the above procedure is that at present there is no previous experience to rely upon in selecting the best way to couple the t_i in S and thus introduce particle correlation. Furthermore, an M-fold integration may be completely intractable from the practical point of view. To overcome these difficulties we shall outline a compact, unified, and quite general method for constructing many-particle correlated trial functions. Recent interest in two-electron trial functions as building blocks for many-electron atomic and molecular wave functions provides a special impetus and makes the method especially topical.

The concept of electron correlation in atoms and molecules is often couched in a spatial geometrical language. Although vague and qualitative, these geometrical concepts have been useful. We shall follow this tradition, but our conceptualization will be in a *precise* geometrical language. Paradoxically, the mathematical *formulation* needed to achieve a measure of geometrical visualization is fairly sophisticated. However, we hasten to point out that no intricate mathematical *manipulation* will ever be necessary.

We shall consider some aspects of the theory of generalized functions concentrated on manifolds of dimension less than N, imbedded in an N-dimensional space. We adhere closely to the discussion in Gel'fand and Shilov.[7]

The most general correlated N-particle trial function we propose can be represented in the following concise form:

$$\Psi(\vec{x}) = \int \delta(P_1, P_2, \cdots, P_k) S(\vec{t}) \varphi(\vec{t}, \vec{x}) d\vec{t}$$
$$\equiv \int_{P_1 = P_2 = \cdots = P_k = 0} S(\vec{t}) \varphi(\vec{t}, \vec{x}) \cdot \omega. \qquad (2)$$

Here the vector $\vec{x}$ designates the set of N *physical* coordinates, while $\vec{t}$ is the collection of the N *nonphysical* integration variables. The volume element $d\vec{t} = dt_1 dt_2 \cdots dt_N$. The Leray form ω of the manifold $P_1 = P_2 = \cdots = P_k = 0$ is defined by[8]

$$dP_1 \cdots dP_k \cdot \omega = d\vec{t}.$$

In particular, if the Jacobian $J(P_1 \cdots P_k / t_1 \cdots t_k) \neq 0$, one may write

$$\omega = dt_{k+1} \cdots dt_N / J.$$

We assume[7] that (1) the $P_i(\vec{t})$ are infinitely differentiable functions and (2) the hypersurfaces $P_i = \mu_i$ ($i = 1, \cdots, k$) form a lattice such that in the neighborhood of every point of the manifold there exists a local coordinate system in which $u_i = P_i(\vec{t})$ for $i = 1, \cdots, k$, and the remaining $u_{k+1}, \cdots, u_N$ can be chosen so that $J(\vec{t}/\vec{u}) > 0$. If $k = 1$, the manifold reduces to a hypersurface ($N-1$ dimensions) and the second condition (now on P_1 only) simply means that there are no singular points on the surface $P_1 = 0$. With the $S(\vec{t})$ in (2) the functional $\Psi(\vec{x})$ is called a *singlet* layer and $S(\vec{t})$, its density. Finally, the generalized function $\delta(P_1, P_2, \cdots, P_k)$ is *defined* by the right-hand side of (2).

Let us now discuss the meaning and significance of the various terms that make up our proposed trial function (2). $\varphi(\vec{t}, \vec{x})$ is our initial, simple approximation to the exact eigenfunction of the Hamiltonian in question. It is the analog of $\varphi_0(xt)$ in (1). The shape function $S(\vec{t})$ is the N-dimensional generalization of $S(t)$ in (1), with the same role. It adjusts $\varphi(\vec{t}, \vec{x})$ to resemble more closely the exact solution. The $P_i(\vec{t})$ are the means by which particle correlation will be introduced. This is achieved by making the P_i depend on more than one nonphysical coordinate t_i. Finally, the role of $\delta(P_1, P_2, \cdots, P_k)$ is to indicate explicitly that because of the k constraints, $P_i = 0$, $i = 1, \cdots, k$, the trial function $\Psi(\vec{x})$ is only an $(N-k)$-fold integral transform.

For the initial approximation $\varphi(\vec{t}, \vec{x})$ we propose the simplest independent-particle function with no adjustable parameters and the t_i as scale factors: $\varphi(\vec{t}, \vec{x}) = \varphi_p(t_1 x_1, t_2 x_2, \cdots, t_N x_N)$. We shall call φ_p a *primitive* function. The reason for this choice is to make integrations with respect to the physical coordinates x_i tractable.

For the shape function $S(\vec{t})$ we recommend a symmetrized product of $S_i(t_i)$. Then, if we choose $P_i(\vec{t}) = t_i$, the optimum product-type $S(\vec{t})$ would reproduce the Hartree-Fock solution.

Notice that the $P_i(\vec{t})$ were chosen to be *independent* of the physical coordinates x_i. Although not essential, this is dictated by practical considerations: $P_i(\vec{t}, \vec{x})$ would make integrations over the x_i intractable. We intend that the physical integrations be performed *first*, followed by the trivial manipulations demanded by the presence of the generalized functions and, if $k < N$, concluded by the $2(N-k)$-fold integration over the remaining t and t' coordinates. (The calculation of expectation values involves integration over the physical coordinates and, if $k < N$, additional integrations in the direct product space $t \times t'$ of the nonphysical coordinates.)

If $N-k$ is small compared with N, we can dispose of the objection against an integral-transform trial function that may be intractable because of high-dimensional integrations.[1] Introducing particle correlation *exclusively* via the $P_i(\vec{t})$ gets rid of the other objection, namely, that we do not know how to couple effectively the t_i in some general form of $S(\vec{t})$. Now at least there is a clear-cut geometrical interpretation to the coupling scheme one decides to choose. By making the t_i scale factors to the corresponding physical coordinates x_i (see the form of φ_p), we can transfer the geometrical interpretation that applies to the nonphysical t space directly to the physical x space. Consequently one can classify now correlated many-particle trial functions in precise geometrical terms by characterizing the correlation-generating $P_i(\vec{t})$.

As these trial functions will be optimized with respect to variational parameters, one has to find a satisfactory answer to the following question: Should one parametrize the P_l, S, or perhaps both? Without some actual experience there is no definite answer at present. One reasonable exploratory program would be the following: Choose for S a delta-convergent sequence and parametrize it; then select a set of P_l that belong to some well-defined class of geometrical objects; finally optimize the parameters with respect to the primitive function φ_p. A very important example of geometrical objects is the class of all hypersurfaces. In particular, the integral of an N-dimensional function $F(\vec{x})$ over the hyperplane $x_1\mu_1+\cdots+x_N\mu_N=p$ is called the Radon transform of $F(\vec{x})$.[9] Its general properties and geometrical meaning are well established.[9]

Assume now that the x_i, $i=1,\cdots,L$, refer to the L electron-nucleus separation coordinates in a molecule. Using Eq. (2) we can construct L-center molecular orbitals that are completely different from the conventional linear combination of atomic orbitals ones and relate much more closely to the geometry of the molecule. Furthermore, the coalescence of the x_l produces a "united-atom" atomic orbital.

We have to discuss the questions of symmetry and statistics. The least sophisticated approach is to construct both the primitive function and the shape function in such a way that they are neither symmetry breaking nor statistics violating. Of course, this also imposes certain restrictions on the arguments of the P_l. Another method would consist of applying symmetrization (and antisymmetrization) operators as well as the appropriate projection operators at the end. The relative merits of these alternatives need further investiastion.

It has to be emphasized that Eq. (2) is not the most general correlated many-particle trial function one could imagine. First, the t_l need not be the scale factors. Second, the $P_l(\vec{t})$ could be made dependent also on the physical coordinates. (This would relate our functions to the more conventional collective-coordinate approach in nuclear physics.[10]) Finally, the general delta function we use could be replaced by an *arbitrary* function of $\vec{x}$ and $\vec{t}$. However, we feel that the formulation we propose combines conceptual simplicity and an appeal to geometrical intuition with the possibility of systematic classification of trial functions and computational practicability.

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π-π PHASE SHIFTS IN THE REGION 1.0-1.4 GeV/c^2 *

B. Y. Oh,† W. D. Walker, J. T. Carroll, M. Firebaugh, A. Garfinkel,‡ and R. Morse
University of Wisconsin, Madison, Wisconsin 53706

and

J. D. Prentice, N. R. Steenberg, and E. West
University of Toronto, Toronto, Canada

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$\pi\pi$ scattering in the di-pion mass region 1.0-1.4 GeV is analyzed. It is shown that an anomaly of the $\pi^-\pi^+$ state in the region 1.0-1.2 GeV is either an $I=0$ D-wave amplitude which interferes with a nearly static $I=1$ P-wave amplitude or a Breit-Wigner D wave which interferes with a moving P wave (possibly resonant). The f^0 meson seems to show considerable inelasticity.

An enhancement in the $\pi^-\pi^+$ mass spectrum in the di-pion mass region 1.0-1.2 GeV has been reported by Whitehead *et al.*,[1] Miller *et al.*,[2] and others.[3] It is noted in Refs. 1 and 2 that the observed enhancement[4] has $I^G=0^+$ and J^P probably 2^+ and is not associated with the S^*, previously