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Geometrization of Quantum Mechanics and the New Interpretation of the Scalar Product in Hilbert Space

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It is shown that the new interpretation of the scalar product in Hilbert space recently proposed by Aharanov, Albert, and Au is in fact the one underlying the stochastic phase-space formulation of nonrelativistic quantum mechanics. The extrapolation of this interpretation to the relativistic domain and its relationship to the program of geometrizing quantum theory and quantizing space-time are discussed.

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In a recently published Letter[1] Aharanov, Albert, and Au have presented a "new" interpretation of the scalar product in Hilbert space. This Letter was soon followed by a Letter of O'Connell and Rajagopal[2] pointing out the equivalence of this interpretation (via recent results by O'Connell and Wigner[3,4]) to Wigner's pioneering work[5] on phase-space distributions in nonrelativistic quantum mechanics. In the present note we intend to point out first, that in fact this "new" interpretation is the one underlying the stochastic phase-space approach to nonrelativistic quantum mechanics,[6,7] and, second, but more important, that this entire approach extends[8] to the relativistic domain, where it leads[9] to a consistent operationally based concept of quantum space-time, or, equivalently, to a new approach to the geometrizing[10-12] of quantum mechanics.

For the sake of simplicity, let us consider only single quantum particles of spin 0. The nonrelativistic quantum mechanics of such particles can be formulated over spaces of exact values, such as the conventional configuration or momentum spaces R^3, as well as[14] over spaces Γ_φ of stochastic phase-space values $(\vec{q},\chi_{\vec{q}})\times(\vec{p},\hat{\chi}_{\vec{p}})$—these last spaces being special cases of Menger-Wald statistical metric spaces.[15] In the former case the measurements of position *or* momentum are assumed to be perfectly accurate, whereas in the second case the measured values are stochastically spread out (so that the uncertainty principle is not violated[7]), and in the optimal cases they represent measurements with extended test particles of normalized proper wave function φ (in the sense of Landé[16] and Born[17]).

Mathematically, these nonrelativistic stochastic phase-space representations can be arrived at by considering[8,9] unitary ray representations of the Galilei group on the Hilbert space $L^2(\Gamma)$ of functions $\psi(\vec{q},\vec{p})$ with inner product

$$\langle\psi_1|\psi_2\rangle=\int_\Gamma\psi_1^*(\vec{q},\vec{p})\psi_2(\vec{q},\vec{p})d^3q\,d^3p\,. \tag{1}$$

For a certain choice of gauge,[8] these representations yield the following representation of the canonical commutation relations (CCR's):

$$Q^j = q^j + i\hbar\partial/\partial p_j, \quad P^j = -i\hbar\partial/\partial q^j. \tag{2}$$

Such representations are, however, highly reducible. One method[8] of finding their irreducible components is to construct unitary mappings which take the configuration-space wave function $\psi(\vec{x})$ of a particle into its representative

$$\psi(\vec{q},\vec{p}) = (2\pi\hbar)^{-3/2}\int \exp[-(i/\hbar)\vec{p}\cdot\vec{x}]\varphi^*(\vec{x}-\vec{q})\psi(\vec{x})d^3x \tag{3}$$

in a subspace $L^2(\Gamma_\varphi)$ that carries an irreducible representation of the CCR's in (2). The quantity $|\psi(\vec{q},\vec{p})|^2$ equals the Aharanov *et al.* expression (4) in Ref. 1, but it can be interpreted not merely as a "propensity", but also as a genuine probability density of the stochastic phase space Γ_φ of stochastic values $(\vec{q},\chi_{\vec{q}})\times(\vec{p},\hat{\chi}_{\vec{p}})$ with confidence functions

$$\chi_{\vec{q}}(\vec{x}) = |\varphi(\vec{x}-\vec{q})|^2, \quad \hat{\chi}_{\vec{p}}(\vec{k}) = |\tilde{\varphi}(\vec{k}-\vec{p})|^2. \tag{4}$$

The correctness of this interpretation follows from the marginality properties[7,14]

$$\int|\psi(\vec{q},\vec{p})|^2 d^3p = \int|\psi(\vec{x})|^2\chi_{\vec{q}}(\vec{x})d^3x, \tag{5}$$

$$\int|\psi(\vec{q},\vec{p})|^2 d^3q = \int|\tilde{\psi}(\vec{k})|^2\hat{\chi}_{\vec{p}}(\vec{k})d^3k \tag{6}$$

as well as from the existence[18,19] of an associated conserved [for $\varphi(x)$ real rotationally symmetric] probability current

$$\vec{j}(\vec{q}) = \int(\vec{p}/m)|\psi(\vec{q},\vec{p})|^2 d^3p, \tag{7}$$

which in the sharp-point limit $\chi_{\vec{q}}(\vec{x}) \to \delta^3(\vec{x}-\vec{q})$ of pointlike test particles merges in its conventional counterpart,

$$\vec{j}(\vec{q}) \to (\hbar/2im)\{\psi^*(\vec{q})\nabla\psi(\vec{q}) - [\nabla\psi^*(\vec{q})]\psi(q)\} \tag{8}$$

and also from a multitude of other results, as reviewed in Ref. 20 (e.g., some of the O'Connell-Wigner results of Ref. 4 have been previously derived in Ref. 18 within this framework).

The transition[8] to the relativistic regime is achieved within this formalism by simply replacing each nonrelativistic concept by its relativistic counterpart, i.e., replacing the Galilei group by the Poincaré group, nonrelativistic by relativistic phase space [of values (q,p) with q in Minkowski space and p on a mass hyperboloid], nonrelativistic by relativistic CCR's (i.e., RCCR's),

$$[Q^\mu,P^\nu] = -i\hbar g^{\mu\nu}, \quad [Q^\mu,Q^\nu] = [P^\mu,P^\nu] = 0, \tag{9}$$

$\psi(\vec{q},\vec{p})$ by $\psi(q,p)$, etc. This leads to a consistent solution of the localizability problem for relativistic quantum particles—which, by Hegerfeld's theorem,[21] has no consistent solution compatible with sharp localizability and relativistic causality. This in turn leads to a concept of quantum space-time[9] based on stochastic geometries[22] delineated by extended quantum test particles in free fall. In its most recent,[12,13] geometrized version, this approach is based on realizations

$$Q_\mu = -i\hbar\nabla_{\bar{\mu}}, \quad P_\mu = i\hbar\nabla_\mu \tag{10}$$

of the RCCR's in (9) by means of covariant derivatives

$$\nabla_\mu = \partial/\partial q^\mu + \Psi_\mu, \quad \nabla_{\bar{\mu}} = \partial/\partial p^\mu + \Phi_\mu. \tag{11}$$

The above covariant derivatives can incorporate metric as well as gauge aspects that reflect some multiplet structure of quantum test particles. These realizations establish, on one hand, a link[23] with Born's reciprocity theory,[24] thus leading[23,25] to mass formulas that yield linear Regge trajectories,[25] whereas, on the other hand, they are intimately related[13] to stochastic phase-space representations of the Poincaré group when $g^{\mu\nu}$ is the Minkowski metric tensor. These representations are fixed by specific choices of the gauges Φ_μ and Ψ_μ, such as, e.g., the simple choice

$$\Phi_\mu(q,p) = (i/\hbar)q_\mu, \quad \Psi_\mu(q,p) = 0 \tag{12}$$

for a spinless particle without internal isospin structure, which nonrelativistically corresponds to the choice occurring in (2). However, whereas no representations of the Poincaré group can be extrapolated to the generic case of curved space-time, the RCCR's remain meaningful even in that case, and can be used in the realization of coordinate transition amplitudes[9,26]

$$K_{B,A}(q_B,p_B;q_A,p_A) = \int\exp[(i/\hbar)v\cdot(m_Aq_A - m_Bq_B)]\eta_A(v\cdot p_A)\eta_A(v\cdot p_A)\eta_B(v\cdot p_B)\delta(v^2-1)d^4v. \tag{13}$$

The probabilities associated (cf. Ref. 9, p. 37) with these amplitudes correspond to measurements of stochastic position and momentum of an A particle by means of a B particle, rather than by "measuring rods" (with the roles of A and B as "system" and "apparatus" being reversible)—and this is exactly the kind of interpretation considered by Aharanov, Albert, and Au in the concluding paragraph of

Ref. 1. Moreover, if we set in (13) $k = m_A v = m_B v$ and write

$$\tilde{\varphi}(k-p) = (2\pi\hbar)^{3/4}\eta_A(v\cdot p), \quad \tilde{\psi}(k-p) = (2\pi\hbar)^{3/4}\eta_B(v\cdot p), \tag{14}$$

then upon making the transition (as in Ref. 8) to the nonrelativistic regime, we get the nonrelativistic counterpart of (13) for $t_A = t_B$:

$$K_{B,A}(\vec{q}_B,\vec{p}_B;\vec{q}_A,\vec{p}_A) = (2\pi\hbar)^{-3/2}\int \exp[(i/\hbar)(\vec{q}_B-\vec{q}_A)\cdot\vec{k}]\,\tilde{\varphi}(\vec{k}-\vec{p}_A)\tilde{\psi}(\vec{k}-\vec{p}_B)\,d^3k. \tag{15}$$

Comparison with (3) via the use of Fourier transform yields the result (since $\tilde{\varphi}$ and $\tilde{\psi}$ are real and rotationally invariant

$$K_{B,A}(\vec{q}_B,\vec{p}_B;\vec{q}_A,\vec{p}_A) = \psi(\vec{q}_B-\vec{q}_A,\vec{p}_B-\vec{p}_A). \tag{16}$$

Hence $|K_{B,A}|^2$ is a generalization of Eq. (4) in Ref. 1 to three-vectors, whereas Eq. (5) in Ref. 1 can be used as an alternative approach[27] to stochastic phase space, which is based on the Weyl group [the appearance of $\exp(i\alpha\beta/2\hbar)$ in Ref. 1 is due to an alternative choice of gauge, which corresponds to setting in (11) $\Phi_\mu = iq_\mu/2\hbar$, $\Psi_\mu = -ip_\mu/2\hbar$, instead of the values in (12)]. However, $|K_{B,A}|^2$ emerges not as the mere "propensity" of Refs. 1 and 2, but rather as a bona fide probability for two extended particles A and B to be at the relative stochastic distance $\vec{q}_B-\vec{q}_A$ and to exhibit the difference $\vec{p}_B-\vec{p}_A$ in their stochastic momenta. In turn, the systematic introduction of such stochastic values in the expression of measurement results even at the pure theoretical level brings about[14,20] the mathematical realization of Born's fundamental data[28,29] that all of physics (classical as well as quantum) should be formulated exclusively in terms of such values instead of deterministic ones, i.e., that "Statements like 'A quantity x has a completely definite value' ... have no physical meaning ... and must be eliminated" (Reference 29, p. 167). As a by-product of such an approach we can achieve in quantum physics informational completeness,[7,30] i.e., set quantum states in one-to-one correspondence with probability densities over stochastic values—a feature discussed by Aharanov, Albert, and Au in Ref. 1, but previously considered for stochastic phase space as well as spin values by others.[30-32]

In summary, the stochastic phase-space approach to nonrelativistic quantum mechanics is based on realizations, of the CCR's [such as (2)] in the Hilbert space $L^2(\Gamma)$, whose elements $\psi(\vec{q},\vec{p})$ can be interpreted as probability amplitudes, which give rise to conserved probability currents (7). These probability amplitudes and currents correspond to measurements with (stochastically) extended rather than point particles. It is this central fact that distinguishes the stochastic phase space from other phase-space approaches to quantum mechanics, and makes possible its consistent extrapolation to the relativistic regime, where there are no covariant counterparts of such nonrelativistic concepts as position operators, Wigner transform, etc. The stochastic phase-space formulation of relativistic quantum mechanics yields, however, covariant probability densities, covariant as well as conserved probability currents, and covariant phase-space propagators. By incorporating the key ideas of Born's reciprocity theory into this framework one arrives at a geometrized version of relativistic quantum mechanics, which is based on the realizations (10) of RCCR's in terms of covariant derivatives. References 23, 25, 26, 33, and 34 provide a sample of recent new results derived within this framework.

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Localized Symmetry-Adapted Perturbation Theory and a New Tight-Binding Expansion

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A new symmetry-adapted perturbation theory is suggested with the following improved properties: The primitive function is localized, and for Coulomb potentials has only a single cusp; the modified equation has no spurious bound states. A systematic tight-binding perturbation expansion involving only two-center integrals is derived.

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In many branches of physics complex systems are described as consisting of simpler "building blocks," e.g., a molecule or a solid may be treated as built up of single atoms or "cells." In the case of a small overlap between neighboring cells' wave functions, approximations of successively increasing order may be constructed starting from "atomic" orbitals. In the present Letter we develop an approach to such problems using a new formulation of a method used in quantum chemistry[1,2] and in nuclear physics[3] under the names of symmetry-adapted perturbation theory (SAPT) and perturbation theory for projected states, respectively. SAPT is used when the complex system possesses some symmetry (e.g., reflections, translations, identical-particle interchange, etc.). Let P be a projection operator ($P^2=P$, $P^\dagger=P$) onto some representation of the symmetry group of H, where H is the Hamiltonian of the complex system. We have $[P,H]=0$, with $H=T+U$, where T and U are the kinetic and the potential energy operators. The complex system wave function ψ ($H\psi=E\psi$, $P\psi=\psi$) cannot usually be approximated by the solution φ_0 of an "atomic" problem, $H_0\varphi_0=E_0\varphi_0$, $H_0=T+V_0$, where V_0 is an atomic potential. Rather, one needs all the atomic orbitals which are obtained by applying to φ_0 the operations of the symmetry group of H. In SAPT a modified equation is introduced,[1-4] for a "primitive function" φ,

$$(H-E)\varphi=(1-P)F(E,\varphi); \tag{1}$$

φ_0 is expected to be a good approximation to φ, and ψ is obtained from φ by projection ($\psi\propto P\varphi$). There is an extensive literature[1-3,5] on the optimal choice of the functional $F(E,\varphi)$, so that higher-order corrections to φ_0 may be treated by perturbation theory.

The wave function ψ is extended over the whole system, whereas atomic orbitals are centered on particular atoms. The requirement that φ of Eq. (1) be localized, similarly to φ_0, is an obvious

