Orthogonalization Process by Recurrence Relations

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An orthogonalization process is proposed, applicable to spaces which are realizations of abstract Hilbert space. It is simpler than the Gram-Schmidt process. A recurrence relation which orthogonalizes a physical space is proposed and it is shown that the generalized Langevin equation is contained therein. This process serves as a basis for understanding the nature of the dynamic many-body formalism.

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In quantum mechanics one encounters degeneracies, e.g., accidental degeneracy. In such a situation one uses the Gram-Schmidt (GS) orthogonalization process[1] to construct a set of orthogonalized wave functions.[2] The GS process is general. It is applicable to any complete set of a finite or infinite number of linearly independent functions or operators definable in a Hilbert space. By this process one can construct a sequence of orthogonal basis vectors spanning a Hilbert space or its linear manifolds.[3] This idea is also formally used. The theories of Mori[4] and Zwanzig,[5] for example, are built by the Mori-Zwanzig projection-operator technique, which is a formal version of the GS process.

If the dimensionality of a Hilbert space is large, the GS process is computationally impractical. Dynamic theories based on the GS process are inevitably very complex formally if relevant Hilbert spaces are infinite dimensional. Such are some of the disadvantages of the GS process due to its *generality*. For most physical problems, one works in some given Hilbert spaces, so that the generality is not really needed. Thus, by using the GS process in these situations, one is bearing the unnecessary burdens. Also one is *not* taking advantage of properties which specific Hilbert spaces can possibly provide.

I propose here an orthogonalization process by recurrence relations (RR's) for functions and operators. RR's are properties of given Hilbert spaces. Hence this alternative process is not generally applicable. The sacrifice in generality, however, permits a direct and practical way of orthogonalization for a particular Hilbert space. In addition, RR's can be physically meaningful precisely because they represent realizations of an abstract Hilbert space. As an application, we show that the generalized Langevin equation of Mori is contained in RR's.

I. *GS orthogonalization process.*—Given a finite or infinite set of independent vectors $\underline{g}=\{g_1, g_2, \ldots, g_\nu, \ldots\}$ in Hilbert space $\mathcal{S}$, one can define an inner product (X, Y), where $X, Y \subset \mathcal{S}$. If $(g_\nu, g_\mu) \neq 0$ for $\nu \neq \mu$, then $\underline{g}$ is not an orthogonal set. One can construct an orthogonal set $\underline{h}=\{h_1, h_2, \ldots h_\nu, \ldots\}$ in $\mathcal{S}$ from $\underline{g}$ by the GS formula[3]

$$h_1 = g_1, \tag{1a}$$

$$h_\nu = g_\nu - \sum_{\kappa=1}^{\nu-1} (g_\nu, h_\kappa)\hat{h}_\kappa, \quad \nu \geq 2, \tag{1b}$$

where $\hat{h}_\kappa = h_\kappa/(h_\kappa, h_\kappa)$. We note that *whatever is the definition of the inner product* (X, Y), $\underline{h}$ is orthogonal, i.e., $(h_\nu, h_\mu)=0$ if $\nu \neq \mu$. Hence, the GS process is completely general and applies to any Hilbert space $\mathcal{S}$.[6]

II. *Recurrence relation in dynamic space.*—Consider a complete set $\mathcal{A}=\{A^{(0)}, A^{(1)}, A^{(2)}, \ldots, A^{(\nu)}, \ldots\}$ in Hilbert space $\mathcal{S}$, where $A^{(\nu)}=(iL)^\nu A$, $\nu \geq 0$, and $LA=[H, A]$, where H is the Hamiltonian and A is a Hermitian operator.[7] We define the inner product of X and Y in $\mathcal{S}$ as

$$(X, Y) = \beta^{-1}\int_0^\beta d\lambda \langle X(\lambda) Y^\dagger\rangle - \langle X\rangle\langle Y^\dagger\rangle, \tag{2}$$

where β is the inverse temperature $\beta=(\kappa_B T)^{-1}$ the dagger denotes Hermitian conjugation, $X(\lambda) = e^{\lambda H} X e^{-\lambda H}$, and $\langle XY\rangle$ is an ensemble average defined by $\langle XY\rangle = \mathrm{Tr}(e^{-\beta H} XY)/\mathrm{Tr}\, e^{-\beta H}$. For simplicity we shall take $\langle X\rangle = \langle Y^\dagger\rangle = 0$.[8] The inner product implies that for any Hermitian vector $X \subset \mathcal{S}$, $[(iL)^\nu X, (iL)^\mu X]=0$ if $|\nu-\mu|$ is an odd number for any $\nu, \mu \geq 0$. It follows from (2) that $\mathcal{A}$ is not an orthogonal set. The aim is to construct an orthogonal set $\underline{f}=\{f_0, f_1, f_2, \ldots, f_\nu, \ldots\}$ in Hilbert space $\mathcal{S}$ from the nonorthogonal set $\mathcal{A}$. This is equivalent to finding a set of basis vectors spanning $\mathcal{S}_A$, the Hilbert space of A, defined by (2).

I construct f_ν inductively by explicitly using (2). With the initial choice $f_0=A$, we have $f_1=iLf_0$ from (2).[9] Next I construct f_2 by writing $f_2=iLf_1 + x$, where x is to be determined by the orthogonality $(f_0, f_2)=(f_1, f_2)=0$. The first condition

gives $-(f_1, f_1)+(x, f_0)=0$. Since $(f_1, f_1)\neq 0$, $x\neq 0$ and $(x, f_0)\neq 0$. The second condition gives $(x, f_1)=0$ hence $x=cf_0$, where c is a constant.[10] It can be determined from the first orthogonality condition, i.e., $c=(f_1, f_1)/(f_0, f_0)\equiv \Delta_1$. Thus, $f_2=iLf_1+\Delta_1 f_0$. With f_0, f_1, and f_2 now given, I let $f_3=iLf_2+y$, where y is to be determined by the orthogonality, i.e., $(y, f_0)=0$, $-(f_2, f_2)+(y, f_1)=0$, and $(y, f_2)=0$. Hence it follows that $y=df_1$, where $d=(f_2, f_2)/(f_1, f_1)\equiv \Delta_2$ and $f_3=iLf_2+\Delta_2 f_1$.

We shall now obtain a RR for $f_{\nu+1}$ assuming that $\{f_0, f_1, \ldots, f_\nu\}$ are known. Let $f_{\nu+1}=iLf_\nu+x_\nu$, $\nu\geq 0$, where x_ν is to be determined. The orthogonality $(f_{\nu+1}, f_\kappa)=0$ for all $\kappa\leq\nu$ gives $-(f_\nu, f_\nu)+(x_\nu, f_{\nu-1})=0$ and $(x_\nu, f_\kappa)=0$ if $\kappa\leq\nu$ but $\kappa\neq\nu-1$. Evidently, $x_\nu=\Delta_\nu f_{\nu-1}$, $\nu\geq 1$ and $x_0=0$, where the constant Δ_ν can be determined from $\Delta_\nu=(f_\nu, f_\nu)/(f_{\nu-1}, f_{\nu-1})$. Hence, finally we obtain

$$f_{\nu+1}=iLf_\nu+\Delta_\nu f_{\nu-1},\quad \nu\geq 0, \tag{3}$$

with $f_{-1}\equiv 0$ and $\Delta_0\equiv 1$.

Through the above RR (3), a complete orthogonal set $\underline{f}$ can be generated from the nonorthogonal set $\mathfrak{A}$. That is, the RR represents an orthogonalization process for $\mathcal{S}_A$. If the inner product in the GS formula (1) is given by (2), then there is a one-to-one correspondence between the two processes. It is, however, vastly simpler to obtain $\underline{f}$ by the RR than by the GS formula if the dimensions of $\mathcal{S}_A$ are large.[11] The RR is a basic property of $\mathcal{S}_A$. Hence it must be contained in all exact dynamic theories operative in $\mathcal{S}_A$.

III. *Recurrence relation in $\mathcal{L}_2$ space.*—Consider a complete set of nonnegative powers of x, $\underline{x}=\{1, x, x^2, \ldots, x^\nu, \ldots\}$ in a Hilbert space $\mathcal{S}$, where x is a real variable. We define the inner product of X and Y in $\mathcal{S}$ as

$$(X, Y)=\int_{-a}^{a} dx\, w(x)XY, \tag{4}$$

where $w(x)$ is a weight function. For simplicity I shall assume $w(x)$ to be an even function of x. Then, $\underline{x}$ is not an orthogonal set. We can construct an orthogonal set $\underline{p}=\{p_0, p_1, p_2, \ldots, p_\nu, \ldots\}$ in $\mathcal{S}_x$, the Hilbert space of x defined by (4). As in II, I shall construct $\underline{p}$ inductively.

If we choose $p_0=1$, then $p_1=x$ because of (4). Let $p_2=xp_1+q$, where q is to be determined by orthogonality, $(p_1, q)=0$ and $(p_1, p_1)+(p_0, q)=0$. Immediately we can write $q=\alpha p_0$, where α is a constant determinable from the second condition. Hence, $p_2=xp_1+\alpha_1 p_0$, where $\alpha=-(p_1, p_1)/(p_0, p_0)\equiv\alpha_1$. Similarly let $p_3=xp_2+r$, where r is to be determined by orthogonality, $(p_0, r)=(p_2, r)=0$ and $(p_2, p_2)+(p_1, r)=0$. Then $r=\beta p_1$, where $\beta=-(p_2, p_2)/(p_1, p_1)\equiv\alpha_2$. Hence $p_3=xp_2+\alpha_2 p_1$. Now we can obtain a RR for $p_{\nu+1}$ by writing $p_{\nu+1}=xp_\nu+q_\nu$, $\nu\geq 0$, where q_ν is to be determined by orthogonality. The orthogonality $(p_{\nu+1}, p_\kappa)=0$ for $\kappa\leq\nu$ gives $(p_\nu, p_\nu)+(p_{\nu-1}, q_\nu)=0$, and $(p_\kappa, q_\nu)=0$ for $\kappa\leq\nu$ but $\kappa\neq\nu-1$. Hence $q_\nu=\alpha_\nu p_{\nu-1}$, where $\alpha_\nu=-(p_\nu, p_\nu)/(p_{\nu-1}, p_{\nu-1})$. Thus we obtain

$$p_{\nu+1}=xp_\nu+\alpha_\nu p_{\nu-1},\quad \nu\geq 0, \tag{5}$$

with $p_{-1}\equiv 0$ and $\alpha_0\equiv 1$.

Equation (5) is the RR for the classical orthogonal polynomials.[12] It represents an orthogonalization process for $\mathcal{S}_x$, equivalent to the GS process for this space. The space $\mathcal{S}_x$ belongs to the class $\mathfrak{L}_2$.[3]

IV. *Auxiliary recurrence relations.*—Consider $\mathcal{S}_A$, the Hilbert space in which linear-response theory is cast.[8] It is a *realization* of an abstract Hilbert space $\mathcal{S}$.[3] Hence the RR for $\mathcal{S}_A$ can be physically meaningful. The Liouville equation $dA(t)/dt=iLA(t)$ has a formal solution in $\mathcal{S}_A$ which may be expressed as

$$A(t)=\sum_{\nu=0} a_\nu(t) f_\nu, \tag{6}$$

where $\underline{f}=\{f_\nu\}$ is given by the RR (3) and $\underline{a}=\{a_\nu(t)\}$ is a set of time-dependent *real* functions. By our choice $f_0=A$, there is a ready link to dynamic response functions, i.e., $a_0(t)$ represents the standard relaxation function $(A(t), A)/(A, A)$ and the other $a_\nu(t)$'s are relatable to the relaxation of the random force defined by the generalized Langevin equation.[13] Then the boundary condition gives $a_0(0)=1$ and $a_\nu(0)=0$ for $\nu\geq 1$.

By applying (6) to the Liouville equation together with the RR (3), we obtain

$$\Delta_{\nu+1} a_{\nu+1}(t)=-\dot{a}_\nu(t)+a_{\nu-1}(t),\quad \nu\geq 0, \tag{7}$$

where $\dot{a}_\nu(t)=da_\nu(t)/dt$ and $a_{-1}\equiv 0$. I shall term (7) the *auxiliary* RR for $\mathcal{S}_A$. By applying the Laplace transform $\mathcal{T}$ on (7), we obtain

$$1=za_0(z)+\Delta_1 a_1(z), \tag{8a}$$

$$a_{\nu-1}(z)=za_\nu(z)+\Delta_{\nu+1} a_{\nu+1}(z),\quad \nu\geq 1, \tag{8b}$$

where $a_\nu(z)=\mathcal{T}[a_\nu(t)]$. I shall term (8) the *dual* auxiliary RR for $\mathcal{S}_A$. By combining Eqs. (8a) and (8b), we can put $a_0(z)$ in a continued fraction as first given by Mori.[4] Thus the auxiliary RR is an expression for the generalized Langevin equation (GLE) in $\mathcal{S}_A$ (see Sec. V). The occurrence of continued fractions in dynamic many-body theory[14] is attributable to the form of the RR (3), and hence ultimately to the structure $\mathcal{S}_A$.

These RR's for $\mathcal{S}_A$ also provide a prescription for acceptable solutions for the relaxation functions $\underline{a}$. For example, we can at once rule out the classical orthogonal polynomials for $\{a_\nu(z)\}$ since the RR for orthogonal polynomials is not congruent to the dual auxiliary RR.[15] Also, since norms are nonnegative real quantities, $\infty > \Delta_\nu \geq 0$. Thus the auxiliary RR (7) does not admit exponential functions as solutions for $a_0(t)$ (Ref. 16) [or the Lorentzian form for $a_0(z)$] if the Liouville operator L remains rigorously Hermitian on $\mathcal{S}_A$.[17]

V. *Physical applications.*—I now show the connection to the GLE.[13,14] From (8a), we have $a_0(z) = [z + \varphi(z)]^{-1}$, where $a_0(z)$ and $\varphi(z) \equiv \Delta_1 a_1(z)/a_0(z)$ are the Laplace-transformed relaxation and memory functions, respectively. The memory function $\varphi(z)$ can be obtained from (8b) by setting $\nu = 1$, and thereby transformed into a continued fraction in terms of $\{\Delta_\nu\}$, $\nu \geq 2$. The random force $f(t)$ can be shown to be $f(z) = \sum_{\nu=1}^{\infty} [a_\nu(z)/a_0(z)] f_\nu$, where $f(z) = \mathcal{T} f(t)$. Observe that $\varphi(z) = (f(z), f_1)/(f_0, f_0)$. These are precisely the expressions obtained by the projection operator technique.[4,5]

I will next illustrate the utility of this formalism by applying it to a physical problem. Consider a homogeneous many-electron system H placed under an external perturbing field, which is suitably turned off at $t = 0$.[18] For $t > 0$ there will be density fluctuations about the Fermi sea. We can study the time evolution via the GLE by taking the dynamical variable A (Ref. 7) to be the density fluctuation operator ρ_k, where k is the wave vector.[15,16] Then the static density response function is (ρ_k, ρ_k), where the inner product is given by (2). That is, the Hilbert space of ρ_k represents a *physical* realization of $\mathcal{S}_A$. Hence, for this fermion system we can obtain dynamic quantities by the RR's (3), (7), and (8), given $\{\Delta_\nu\}$.

For density fluctuations in two dimensions at $T = 0$ and $k \ll k_F$ (k_F the Fermi wave vector), the Δ's have been calculated by aid of (3),[15] viz., $\Delta_1 = 2\Delta + \Gamma$, $\Delta_\nu = \Delta$ for $\nu \geq 2$, where $\Delta = (k\epsilon_F)^2$ and $\Gamma = 2\pi\rho e^2 k/m$ (ϵ_F the Fermi energy, ρ the electron number density, m mass, e charge). The difference between the ideal and nonideal systems appears only in Δ_1 through Γ. For the ideal system ($\Gamma = 0$) these Δ's imply that the auxiliary RR (7) is just the RR for the Bessel functions J_ν. Hence, $a_\nu(t) = (\frac{1}{2}\mu)^{-\nu} J_\nu(\mu t)$, $\nu \geq 0$, and $\mu = 2\Delta^{1/2}$. One can also obtain $a_0(z)$ by (8) and $a_0(t)$ by $\mathcal{T}^{-1} \times a_0(z)$, and hence $a_\nu(t)$, $\nu \geq 1$, by (7).[16] Thus,

$$\rho_k(t) = \sum_{\nu=0}^{\infty} [(\tfrac{1}{2}\mu)^{-\nu} J_\nu(\mu t)] f_\nu$$

and

$$f(t) = \sum_{\nu=1}^{\infty} [(\tfrac{1}{2}\mu)^{-\nu+1} 2\nu J_\nu(\mu t)/\mu t] f_\nu,$$

where $\{f_\nu\}$ is given by (3) with $f_0 = \rho_k$.

For the nonideal system ($\Gamma \neq 0$) it is also possible to obtain an analytic solution for $a_0(t)$ by (8), and hence $a_\nu(t)$, $\nu \geq 1$, by (7). For density fluctuations in three dimensions I have similarly obtained dynamic solutions. I have also successfully applied this formalism to obtain critical dynamics of the spin-$\frac{1}{2}$ van der Waals model.[19] Solutions to these problems will be given elsewhere. Our formal method appears to have possible applications to a variety of time-dependent many-body problems.

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[1]J. P. Gram, Z. Math. 94, 41 (1883); E. Schmidt, Math. Ann. 63, 442 (1907).

[2]See E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1961).

[3]See N. I. Akhiezer and I. M. Glazman, *Theory of Linear Operators in Hilbert Space* (Ungar, New York, 1961), Vols. 1 and 2.

[4]H. Mori, Prog. Theor. Phys. 34, 399 (1965).

[5]R. Zwanzig, J. Chem. Phys. 33, 1338 (1960); S. Nordholm and R. Zwanzig, J. Stat. Phys. 13, 347 (1975).

[6]The GS formula (1) constructs h_ν inductively, i.e., $\{h_1, h_2, \ldots, h_{\nu-1}\}$ are assumed known. The initial choice $h_1 = g_1$ is arbitrary. But it is also crucial since all other h's now depend on it and there is no more room for arbitrariness. The initial one degree of freedom allows some interesting physical possibilities. In quantum mechanical applications, $\underline{g}$ may be a set of independent wave functions which are mutually not orthogonal because of some degeneracies. A new set $\underline{h}$ is then composed of only orthogonalized wave functions. See Ref. 2 (pp. 145 and 314) for specific examples.

[7]Here A may be a quantum mechanical operator, e.g., the total spin operator ($s = \frac{1}{2}$). Such an operator will be referred to as a dynamical variable or a vector in a Hilbert space. The Liouville operator L is a linear Hermitian operator defined on a Hilbert space.

[8]The inner product (2) is used in statistical mechanics. See, for example, H. Falk and L. W. Bruch, Phys. Rev. 180, 442 (1969); M. Suzuki, Physica (Utrecht) 51, 277 (1971); I. M. Kim and M. H. Lee, Phys. Rev. B 24, 3961 (1981). Also see N. Mermin and H. Wagner, Phys. Rev. Lett. 17, 1133 (1966); J. Naudts and A. Verbeure, J. Math. Phys. (N.Y.) 17, 419 (1976); F. J. Dyson, E. H. Lieb, and B. Simon, J. Stat. Phys. 18, 335

(1978). The origin of this inner product may be traced to linear-response theory. See R. Kubo, in *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience, New York, 1959), Vol. 1. One may regard $X(\lambda)$ as the "temperature evolution" of X since $X(\lambda = it)$, where t is time, represents the temporal development of X in the Heisenberg picture. See the first three references here.

[9]This initial choice is natural especially for making a connection to linear-response theory. For developing nonlinear-response theories, some other choice might be preferable, which is permitted by the arbitrariness of the initial choice.

[10]One can also take $x = c'(iL)^2 f_0$, which also satisfies $(x, f_1) = 0$. But this choice gives $c' = -1$, hence $f_2 = 0$, which contradicts completeness.

[11]The complexity of the direct application of the GS procedure (1b) may be apparent if one tries to write down $\{h_\kappa\}$ in terms of $\{g_\kappa\}$, $1 \leq \kappa \leq \nu$, for say $\nu = 5$. As κ becomes larger, it rapidly gets out of hand. The reason is that they must each be independently calculated and they become progressively more laborious. For a glimpse into the complexity, see Mori, Ref. 4, where a few examples are shown. In contrast, the new procedure (3) enables one to obtain a given f_κ from the previously obtained lower-dimensional f's. Hence it is efficient and especially suited for calculating the norms (f_κ, f_κ). See Sec. V.

[12]Most classical orthogonal polynomials have an even weight function $w(x)$ and a symmetric interval $(-a, a)$. The exceptions are the Jacobi and Laguerre polynomials. For the cases with a noneven weight function and a nonsymmetric interval, the RR is slightly changed. It is still a three-term relation with only the coefficient of P_ν in (5) shifted, i.e., $x \to x + \beta_\nu$, where β_ν is a constant. See G. Szegö, *Orthogonal Polynomials* (American Mathematical Society, Providence, Rhode Island, 1975). The RR is usually regarded as a result deduced from certain differential equations bearing the names of these polynomials. What we have shown is that it is a property of $\mathcal{S}_x$, deducible directly from the definition of the inner product. See S. Bocher, Math. Z. 29, 730 (1929); P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), pp. 541–557.

[13]H. Mori, Prog. Theor. Phys. 33, 423 (1965); M. H. Lee, Phys. Rev. B 26, 2547 (1982).

[14]See S. Lovesey, *Dynamic Correlations* (Benjamin, Reading, Mass., 1980).

[15]For example, the RR for the Bessel function is contruent to Eq. (7). See M. H. Lee and J. Hong, Phys. Rev. Lett. 48, 634 (1982).

[16]Note that one needs to determine only $a_0(t)$ since all other relaxation functions follow by the auxiliary RR.

[17]R. Kubo, in *Transport Phenomena*, edited by G. Kirczenow (Springer, Berlin, 1974), pp. 123-4. The Lorentzian form gives rise to central peaks in frequency spectra obtained by, e.g., inelastic scattering of neutrons in liquids and magnets, collectively referred to as the central-peak problem. Most of the approximations employed in the central-peak problem are mathematically untenable. Their "spaces" have, for example, complex norms and arbitrary dimensions (usually three), which bear no relationship to the structure of $\mathcal{S}_A$.

[18]For H we use a model due to K. Sawada, Phys. Rev. 106, 372 (1957). It is a useful model for high-density electronic systems whose excitations are limited largely to electron-hole scattering near the Fermi sea. Recent experimental studies of inversion and accumulation layers of the metal-oxide-semiconductors have stimulated considerable interest in two-dimensional many-electron models. See T. Ando *et al.*, Rev. Mod. Phys. 54, 437 (1982).

[19]R. Dekeyser and M. H. Lee, Phys. Rev. B 19, 265 (1979). M. H. Lee, J. Math. Phys. 23, 464 (1982).