

Nonperturbational “Continued-Fraction” Spin-offs of Quantum Theory’s Standard Perturbation Methods

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Abstract

The inherently homogeneous stationary-state and time-dependent Schrödinger equations are often recast into inhomogeneous form in order to resolve their solution nonuniqueness. The inhomogeneous term can impose an initial condition or, for scattering, the preferred permitted asymptotic behavior. For bound states it provides sufficient focus to exclude all but one of the homogeneous version’s solutions. Because of their unique solutions, such inhomogeneous versions of Schrödinger equations have long been the indispensable basis for a solution scheme of successive perturbational corrections which are anchored by their inhomogeneous term. Here it is noted that every such perturbational solution scheme for an inhomogeneous linear vector equation spins off a nonperturbational continued-fraction scheme. Unlike its representation-independent antecedent, the spin-off scheme only works in representations where all components of the equation’s inhomogeneous term are nonzero. But that requirement seems to confer theoretical physics robustness heretofore unknown: for quantum fields the order of the perturbation places a bound on unperturbed particle number, the spin-off scheme contrariwise has only basis elements of unbounded unperturbed particle number. It furthermore is difficult to visualize such a continued-fraction spin-off scheme generating infinities, since its successive iterations always go into denominators.

Introduction

Schrödinger equations, whether stationary-state or time-dependent, are homogeneous, and as such can suffer from solution nonuniqueness. In order to be able to effectively apply standard successive approximation schemes, such as perturbational ones, to Schrödinger equations, they are often first recast into a specialized *inhomogeneous* linear form which has a *unique* solution. Denoting its state vector as $|\psi\rangle$, a simple generic presentation of a Schrödinger equation in inhomogeneous form is,

$$|\psi\rangle = |\psi_0\rangle - \widehat{\mathcal{V}}|\psi\rangle. \quad (1a)$$

The state vector $|\psi_0\rangle$, which comprises the *inhomogeneous term* of Eq. (1a) usually shares a *key feature* with $|\psi\rangle$, such as asymptotic behavior in a region of infinite extent or exact value at an initial time, or, alternately, *is a passable approximation to $|\psi\rangle$* . Given that the Hamiltonian operator of the homogeneous Schrödinger equation which underlies Eq. (1a) is \widehat{H} , we *in addition* assume the existence of an *exactly diagonalizable Hamiltonian operator* \widehat{H}_0 that has $|\psi_0\rangle$ as one of its *eigenstates*, and for which the linear operator $\widehat{\mathcal{V}}$ of Eq. (1a) is of no less than *first order in $\widehat{\mathcal{V}} \stackrel{\text{def}}{=} (\widehat{H} - \widehat{H}_0)$* .

If we now take the viewpoint that the inhomogeneous term $|\psi_0\rangle$ on the right-hand side of Eq. (1a) is a sufficiently good approximation to $|\psi\rangle$ on its left-hand side that the remainder term $-\widehat{\mathcal{V}}|\psi\rangle$ *is only a small perturbation*, then the *perturbational successive approximations*,

$$|\psi^{(n+1)}\rangle = |\psi_0\rangle - \widehat{\mathcal{V}}|\psi^{(n)}\rangle, \quad (1b)$$

where, of course, $|\psi^{(0)}\rangle = |\psi_0\rangle$, would be expected to converge reasonably rapidly.

Additional insight into the Eq. (1b) *perturbational iteration scheme* can be obtained from taking the second term on the right-hand side of Eq. (1a) to its left-hand side, which yields,

$$|\psi\rangle + \widehat{\mathcal{V}}|\psi\rangle = |\psi_0\rangle. \quad (1c)$$

Eq. (1c) has the formal operator solution,

$$|\psi\rangle = [1 + \widehat{\mathcal{V}}]^{-1}|\psi_0\rangle. \quad (1d)$$

This presents the issue of how to practically evaluate the formal operator $[1 + \widehat{\mathcal{V}}]^{-1}$. One way is to try to use its formal geometric series expansion,

$$[1 + \widehat{\mathcal{V}}]^{-1} = 1 - \widehat{\mathcal{V}} + (\widehat{\mathcal{V}})^2 + \cdots + (-\widehat{\mathcal{V}})^n + \cdots, \quad (1e)$$

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which is readily verified to yield the exactly the same result when inserted into Eq. (1d) as is obtained from successively applying the Eq. (1b) perturbational iteration scheme. Given the well-known convergence and divergence characteristics of the geometric series, it is apparent that the Eq. (1b) perturbational iteration scheme for the inhomogeneous Eq. (1a) *is unlikely to be greatly useful unless $|\psi_0\rangle$ is substantially dominant over $\widehat{\mathcal{V}}|\psi_0\rangle$.*

That naturally raises the question of whether there might be an *alternate* general iteration approach to the inhomogeneous Eq. (1a) that could come to the rescue when its Eq. (1b) *perturbational* iterations converge too slowly or diverge. A Lippmann-Schwinger nonrelativistic potential-scattering variant of the inhomogeneous Eq. (1a), considered for *arbitrarily strong* potentials in a recent article [1], has revealed that *if* a complete representation basis set $\{\langle\rho_i|\}$ can be found such that *every component* $\langle\rho_i|\psi_0\rangle$ of the inhomogeneous-term state vector $|\psi_0\rangle$ *is nonzero*, then a robust nonperturbational iteration scheme can be devised from *the explicit presentation of* Eq. (1c) *in that representation*, namely from the specific equalities,

$$\langle\rho_i|\psi\rangle + \langle\rho_i|\widehat{\mathcal{V}}|\psi\rangle = \langle\rho_i|\psi_0\rangle. \quad (2a)$$

If we now make the *assumption* that $\langle\rho_i|\psi\rangle$ is, like $\langle\rho_i|\psi_0\rangle$, *nonzero*, we can *factor the left-hand side of* Eq. (2a) into $\langle\rho_i|\psi\rangle$ and *the resulting nonzero cofactor*. We then proceed to *divide both sides of* Eq. (2a) *by that nonzero cofactor*, which changes the appearance of Eq. (2a) to,

$$\langle\rho_i|\psi\rangle = \langle\rho_i|\psi_0\rangle / \left[1 + (\langle\rho_i|\psi\rangle)^{-1} \langle\rho_i|\widehat{\mathcal{V}}|\psi\rangle \right], \quad (2b)$$

from which we straightforwardly devise the manifestly nonperturbational successive-approximation scheme,

$$\langle\rho_i|\psi^{(n+1)}\rangle = \langle\rho_i|\psi_0\rangle / \left[1 + (\langle\rho_i|\psi^{(n)}\rangle)^{-1} \langle\rho_i|\widehat{\mathcal{V}}|\psi^{(n)}\rangle \right], \quad (2c)$$

where, of course, $\langle\rho_i|\psi^{(0)}\rangle = \langle\rho_i|\psi_0\rangle$. If $\langle\rho_i|\psi^{(n)}\rangle$ is nonzero, then because $\langle\rho_i|\psi_0\rangle$ is nonzero, barring the pathological occurrence of a divergence in $\langle\rho_i|\widehat{\mathcal{V}}|\psi^{(n)}\rangle$, $\langle\rho_i|\psi^{(n+1)}\rangle$ will in turn be nonzero. We also note that the iteration scheme of Eq. (2c) has the desirable nonperturbational character of a *continued fraction*.

Thus the Eq. (1a) generic specialized *inhomogeneous* form of the Schrödinger equation *always* spawns *not only* the perturbational successive-approximation scheme of Eq. (1b), but *as well* the nonperturbational continued-fraction successive-approximation scheme of Eq. (2c) that can regarded as its spin-off.

We shall now survey some of the well-known circumstances where a Schrödinger equation with Hamiltonian operator \widehat{H} for a state $|\psi\rangle$ is combined *both* with a *state* $|\psi_0\rangle$ which has a crucial similarity to $|\psi\rangle$ *and as well* with an exactly diagonalizable *Hamiltonian operator* \widehat{H}_0 that includes $|\psi_0\rangle$ as one of its eigenstates to produce an *inhomogeneous* linear equation for $|\psi\rangle$ *which has the generic form given by* Eq. (1a), where the linear operator $\widehat{\mathcal{V}}$ is of at least first order in $\widehat{\mathcal{V}} \stackrel{\text{def}}{=} (\widehat{H} - \widehat{H}_0)$. We shall as well mention some of the complete *representation basis sets* $\{\langle\rho_i|\}$ for which certain of the surveyed inhomogeneous terms $|\psi_0\rangle$ have *exclusively nonzero components* $\langle\rho_i|\psi_0\rangle$ —note that the *eigenstate set* of the Hamiltonian operator \widehat{H}_0 is *entirely unacceptable* as such a complete representation basis set $\{\langle\rho_i|\}$ because *all* of its members *aside from* $\langle\psi_0|$ *itself* are *orthogonal to* $|\psi_0\rangle$.

The Lippmann-Schwinger equation for nonrelativistic potential scattering

As in Ref. [1] we consider the coordinate-representation nonrelativistic Schrödinger equation for an eigenstate $\langle\mathbf{r}|\psi_E\rangle$ of *positive energy* E ,

$$\left(-\hbar^2\nabla_{\mathbf{r}}^2/(2m) + V(\mathbf{r})\right) \langle\mathbf{r}|\psi_E\rangle = E\langle\mathbf{r}|\psi_E\rangle, \quad (3a)$$

where,

$$\lim_{|\mathbf{r}|\rightarrow\infty} V(\mathbf{r}) = 0. \quad (3b)$$

Thus for sufficiently large $|\mathbf{r}|$, the Schrödinger equation of Eq. (3a) reduces to,

$$\left(-\hbar^2\nabla_{\mathbf{r}}^2/(2m)\right) \langle\mathbf{r}|\psi_E\rangle = E\langle\mathbf{r}|\psi_E\rangle, \quad (3c)$$

which is satisfied by *any plane wave* $e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$ for which $|\mathbf{p}| = (2mE)^{\frac{1}{2}}$ and by *any linear superposition* of these plane waves. Among those linear superpositions are all the angularly modulated ingoing and outgoing *spherical waves* that have wave number $k = (2mE)^{\frac{1}{2}}/\hbar$.

Now a *scattering experiment* at energy $E > 0$ is described by a *particular solution* of the Schrödinger Eq. (3a) which at sufficiently large $|\mathbf{r}|$ that Eq. (3a) is well-approximated by Eq. (3c) consists of only a *single* specified plane wave $e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$ of momentum \mathbf{p} plus *only outgoing* spherical waves [2]. We denote this *scattering solution* of the Schrödinger Eq. (3a) as $\langle \mathbf{r} | \psi_{\mathbf{p}}^+ \rangle$.

It turns out that an *inhomogeneous modification* of the Schrödinger Eq. (3a) describes $\langle \mathbf{r} | \psi_{\mathbf{p}}^+ \rangle$ *uniquely*, namely the following nonrelativistic Lippmann-Schwinger equation for potential scattering [2],

$$\langle \mathbf{r} | \psi_{\mathbf{p}}^+ \rangle = e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} - \langle \mathbf{r} | (\hat{H}_0 - E_{\mathbf{p}} - i\epsilon)^{-1} \hat{V} | \psi_{\mathbf{p}}^+ \rangle, \quad (3d)$$

where $\hat{H}_0 \stackrel{\text{def}}{=} |\hat{\mathbf{p}}|^2/(2m) = -\hbar^2 \hat{\nabla}^2/(2m)$ is the kinetic energy *operator* and $E_{\mathbf{p}} \stackrel{\text{def}}{=} |\mathbf{p}|^2/(2m)$ is the kinetic energy *c-number scalar* that corresponds to the c-number momentum vector \mathbf{p} .

Taking $\langle \mathbf{r} | \mathbf{p} \rangle \stackrel{\text{def}}{=} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$, we can write Eq. (3d) in the form of Eq. (1a), i.e.,

$$|\psi_{\mathbf{p}}^+ \rangle = |\mathbf{p} \rangle - (\hat{H}_0 - E_{\mathbf{p}} - i\epsilon)^{-1} \hat{V} |\psi_{\mathbf{p}}^+ \rangle, \quad (3e)$$

where $|\psi_0 \rangle = |\mathbf{p} \rangle$ and $\hat{V} = (\hat{H}_0 - E_{\mathbf{p}} - i\epsilon)^{-1} \hat{V}$. Furthermore, since $\hat{H}_0 |\mathbf{p} \rangle = E_{\mathbf{p}} |\mathbf{p} \rangle$, we can recover the Schrödinger Eq. (3a) from Eq. (3e) by multiplying the latter through by $(\hat{H}_0 - E_{\mathbf{p}})$, followed by rearrangement of the resulting terms between the left-hand and right-hand sides.

The negative imaginary infinitesimal $-i\epsilon$ that appears in the Lippmann-Schwinger Eqs. (3d) and (3e) ensures that *only outgoing* spherical waves are present for sufficiently large $|\mathbf{r}|$, in *addition*, of course, to the *single* specified plane wave $e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$ of momentum \mathbf{p} .

The usual *perturbational iteration* of the Lippmann-Schwinger Eq. (3d) is,

$$\langle \mathbf{r} | \psi_{\mathbf{p}}^{(n+1)+} \rangle = e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} - \langle \mathbf{r} | (\hat{H}_0 - E_{\mathbf{p}} - i\epsilon)^{-1} \hat{V} | \psi_{\mathbf{p}}^{(n)+} \rangle, \quad (3f)$$

which with $\langle \mathbf{r} | \psi_{\mathbf{p}}^{(0)+} \rangle = e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$ generates the familiar perturbational geometric *Born series* for nonrelativistic potential scattering [3].

For *nonperturbational* “continued-fraction” iteration of the Lippmann-Schwinger Eq. (3d) we happen to be in the extraordinarily fortunate situation that *coordinate representation* of the inhomogeneous term $|\psi_0 \rangle = |\mathbf{p} \rangle$ is *always nonzero* because $\langle \mathbf{r} | \mathbf{p} \rangle = e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \neq 0$. Therefore in the manner of Eq. (1c) and Eqs. (2a)–(2c), the Lippmann-Schwinger Eq. (3d) in coordinate representation gives rise to the nonperturbational “continued fraction” iteration scheme,

$$\langle \mathbf{r} | \psi_{\mathbf{p}}^{(n+1)+} \rangle = e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} / \left[1 + \left(\langle \mathbf{r} | \psi_{\mathbf{p}}^{(n)+} \rangle \right)^{-1} \langle \mathbf{r} | (\hat{H}_0 - E_{\mathbf{p}} - i\epsilon)^{-1} \hat{V} | \psi_{\mathbf{p}}^{(n)+} \rangle \right], \quad (3g)$$

where we of course have that $\langle \mathbf{r} | \psi_{\mathbf{p}}^{(0)+} \rangle = e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$.

A bound-state inhomogeneous equation suitable for iteration solution

The just-discussed Lippmann-Schwinger equation is an *inhomogeneous* Schrödinger-equation variant that is of the form of our generic Eq. (1a). With an arbitrary plane wave as its *inhomogeneous term*; the Lippmann-Schwinger equation enables *completely prescribed iteration refinement* of that approximating plane wave toward its *unique* associated “asymptotically outgoing-only spherical-wave” *exact* scattering wave function. The *key ingredient* that is needed to fashion the *inhomogeneous* Lippmann-Schwinger equation from its underlying *homogeneous* Schrödinger equation is of course the “outgoing-only spherical-wave” free-particle propagator, which is constructed from the *selfsame* free-particle Hamiltonian for which that approximating plane wave *is an eigenstate*.

In contrast, the *standard* Schrödinger approach to the perturbational refinement of an approximating *bound state* $|\psi_j^0 \rangle$ fails to *explicitly present* the *inhomogeneous* Schrödinger-equation variant which *links* that approximating bound state to a *unique* associated *exact* bound-state solution $|\psi_j \rangle$ of the underlying homogeneous stationary-state Schrödinger equation $\hat{H} |\psi_j \rangle = E_j |\psi_j \rangle$. Due to the *absence* of the information which is *inherent* to that *inhomogeneous linking equation*, the standard Schrödinger bound-state perturbational approach *can't offer minutely prescribed iteration instructions* for its perturbational refinement procedure [4]. More importantly, if that inhomogeneous linking equation is *not* in hand, there is no obvious way to devise alternate *nonperturbational* methods for the iteration refinement of approximating bound states.

Fortunately, we can follow the blueprint that is provided to us by the Lippmann-Schwinger equation to devise its missing bound-state analog. A *major difference* between the two, however, is that bound states

certainly *don't* feature outgoing, ingoing or *any other type of traveling wave*. Therefore the kind of propagator we need for bound states is of the *standing-wave* type. Nor can a propagator suited to an approximating *bound state* possibly be constructed from the *free-particle* Hamiltonian operator as it *properly is* for the approximating *plane waves* of the Lippmann-Schwinger equation. The construction of the *standing wave* propagator we need must be from a Hamiltonian operator \widehat{H}_0 which has that *approximating bound state* $|\psi_j^0\rangle$ as one of its *bound-state eigenstates*, i.e., \widehat{H}_0 must satisfy,

$$\widehat{H}_0|\psi_j^0\rangle = E_j^0|\psi_j^0\rangle. \quad (4a)$$

Of course, since that approximating bound state $|\psi_j^0\rangle$ is indeed *bound*, we can *normalize it to unity*, i.e.,

$$\langle\psi_j^0|\psi_j^0\rangle = 1. \quad (4b)$$

Finally, the *construction* of the required standing-wave propagator from the Hamiltonian operator \widehat{H}_0 *can't be accomplished in practice unless \widehat{H}_0 is exactly diagonalizable*. If all the eigenstates and eigenvalues of \widehat{H}_0 are *actually available*, its corresponding standing-wave propagator can be obtained in the schematic form,

$$\left[P/(\widehat{H}_0 - E_j^0)\right] \stackrel{\text{def}}{=} \lim_{\epsilon \rightarrow 0} \left(\widehat{H}_0 - E_j^0\right) \left[\left(\widehat{H}_0 - E_j^0\right)^2 + \epsilon^2\right]^{-1} = \sum_{i \neq j} |\psi_i^0\rangle\langle\psi_i^0|/(E_i^0 - E_j^0), \quad (4c)$$

where the letter P in the standing-wave propagator's definition denotes "principal value". The exactly diagonalizable Hamiltonian operator \widehat{H}_0 is frequently called the "unperturbed" Hamiltonian operator, its particular bound eigenstate $|\psi_j^0\rangle$ the "unperturbed" approximating bound state, and that state's \widehat{H}_0 eigenvalue E_j^0 the corresponding "unperturbed" approximating bound-state energy. By the same token, one could call the operator $\left[P/(\widehat{H}_0 - E_j^0)\right]$ the "unperturbed" standing-wave propagator. Note that $\left[P/(\widehat{H}_0 - E_j^0)\right]$ has a special feature *which has no analog for traveling-wave propagators* such as the outgoing-wave propagator of the Lippmann-Schwinger equation, namely that,

$$\langle\psi_j^0| \left[P/(\widehat{H}_0 - E_j^0)\right] = 0. \quad (4d)$$

The final ingredient we need to obtain the bound-state analog of the inhomogeneous Lippmann-Schwinger equation is the homogeneous stationary-state Schrödinger equation for the *exact* bound state $|\psi_j\rangle$ that is *uniquely linked* to the "unperturbed" approximating bound state $|\psi_j^0\rangle$. Denoting the *exact* Hamiltonian operator for the physical system we are studying as \widehat{H} , this homogeneous stationary-state Schrödinger equation is of course,

$$\widehat{H}|\psi_j\rangle = E_j|\psi_j\rangle,$$

which it can sometimes be more convenient to express as,

$$\left[\widehat{H} - E_j\right] |\psi_j\rangle = 0.$$

Since the physical system's *exact* Hamiltonian operator \widehat{H} *won't* in general be exactly diagonalizable (*unlike* the somewhat artificial "unperturbed" Hamiltonian operator \widehat{H}_0), we have no more a priori knowledge of the particular *exact* bound-state *energy* E_j than we do of its corresponding *exact* bound-state eigenstate $|\psi_j\rangle$ of the exact Hamiltonian operator \widehat{H} . In order to *avoid* having the exact bound-state energy E_j become a *completely independent unknown for which we need to solve*, we choose to write the physical system's exact homogeneous stationary-state Schrödinger equation for the bound state $|\psi_j\rangle$ in the more cumbersome form,

$$\left[\widehat{H} - \left(\langle\psi_j|\widehat{H}|\psi_j\rangle/\langle\psi_j|\psi_j\rangle\right)\right] |\psi_j\rangle = 0, \quad (4e)$$

which *entirely supplants* E_j by $|\psi_j\rangle$ and \widehat{H} .

Eqs. (4a)–(4e) supply all the ingredients needed to devise the bound-state analog of the Lippmann-Schwinger equation. Inspection of the Lippmann-Schwinger equation strongly suggests that we multiply the physical system's homogeneous Schrödinger Eq. (4e) from the left by the "unperturbed" standing-wave

propagator $\left[P/(\widehat{H}_0 - E_j^0) \right]$ as the first step toward that analog. That operator multiplication produces the physical Schrödinger-equation variant,

$$\left[P/(\widehat{H}_0 - E_j^0) \right] \left[\widehat{H} - \left(\langle \psi_j | \widehat{H} | \psi_j \rangle / \langle \psi_j | \psi_j \rangle \right) \right] |\psi_j\rangle = 0, \quad (4f)$$

which is not yet the *inhomogeneous* Lippmann-Schwinger equation analog that we seek. To complete our task we now develop an *identity* involving $|\psi_j\rangle$, $\left[P/(\widehat{H}_0 - E_j^0) \right]$ and $\left[-\widehat{H}_0 + E_j^0 \right]$ to which we shall then *add* the Eq. (4f) physical Schrödinger-equation variant. One might naively expect that,

$$|\psi_j\rangle + \left[P/(\widehat{H}_0 - E_j^0) \right] \left[-\widehat{H}_0 + E_j^0 \right] |\psi_j\rangle = 0,$$

but if we multiply the left-hand side of this proposed equality by $\langle \psi_j^0 |$ and take note of Eq. (4d), we see that the result is $\langle \psi_j^0 | \psi_j \rangle$ rather than zero. From Eqs. (4c) and (4b) it is indeed seen that,

$$|\psi_j\rangle + \left[P/(\widehat{H}_0 - E_j^0) \right] \left[-\widehat{H}_0 + E_j^0 \right] |\psi_j\rangle = |\psi_j^0\rangle \langle \psi_j^0 | \psi_j \rangle. \quad (4g)$$

We now add the Eq. (4g) *identity* to the physical Schrödinger-equation variant given by Eq. (4f) to obtain,

$$|\psi_j\rangle + \left[P/(\widehat{H}_0 - E_j^0) \right] \left[\widehat{H} - \widehat{H}_0 + E_j^0 - \left(\langle \psi_j | \widehat{H} | \psi_j \rangle / \langle \psi_j | \psi_j \rangle \right) \right] |\psi_j\rangle = |\psi_j^0\rangle \langle \psi_j^0 | \psi_j \rangle. \quad (4h)$$

If we now define the “interaction Hamiltonian operator” \widehat{V} as,

$$\widehat{V} \stackrel{\text{def}}{=} (\widehat{H} - \widehat{H}_0), \quad (4i)$$

we can rewrite Eq. (4h) as,

$$|\psi_j\rangle + \left[P/(\widehat{H}_0 - E_j^0) \right] \left[\widehat{V} - \left(\langle \psi_j | (\widehat{V} + \widehat{H}_0 - E_j^0) | \psi_j \rangle / \langle \psi_j | \psi_j \rangle \right) \right] |\psi_j\rangle = |\psi_j^0\rangle \langle \psi_j^0 | \psi_j \rangle. \quad (4j)$$

If we move the term involving the “unperturbed” standing-wave propagator $\left[P/(\widehat{H}_0 - E_j^0) \right]$ to the right-hand side of Eq. (4j), we obtain,

$$|\psi_j\rangle = |\psi_j^0\rangle \langle \psi_j^0 | \psi_j \rangle - \left[P/(\widehat{H}_0 - E_j^0) \right] \left[\widehat{V} - \left(\langle \psi_j | (\widehat{V} + \widehat{H}_0 - E_j^0) | \psi_j \rangle / \langle \psi_j | \psi_j \rangle \right) \right] |\psi_j\rangle, \quad (4k)$$

which is the inhomogeneous bound-state analog of the Lippmann-Schwinger equation presented in Eq. (3e). The exact energy E_j of the exact physical bound state $|\psi_j\rangle$ is of course given by,

$$E_j = \left(\langle \psi_j | (\widehat{V} + \widehat{H}_0) | \psi_j \rangle / \langle \psi_j | \psi_j \rangle \right). \quad (4l)$$

The complete detailed prescription for the *perturbational iteration* of Eq. (4k) is then obviously,

$$|\psi_j^{(n+1)}\rangle = |\psi_j^0\rangle \langle \psi_j^0 | \psi_j^{(n)}\rangle - \left[P/(\widehat{H}_0 - E_j^0) \right] \left[\widehat{V} - \left(\langle \psi_j^{(n)} | (\widehat{V} + \widehat{H}_0 - E_j^0) | \psi_j^{(n)}\rangle / \langle \psi_j^{(n)} | \psi_j^{(n)}\rangle \right) \right] |\psi_j^{(n)}\rangle, \quad (4m)$$

where, of course, $|\psi_j^{(0)}\rangle = |\psi_j^0\rangle$. In addition, *entirely as a byproduct of* $|\psi_j^{(n)}\rangle$, we have,

$$E_j^{(n+1)} = \left(\langle \psi_j^{(n)} | (\widehat{V} + \widehat{H}_0) | \psi_j^{(n)}\rangle / \langle \psi_j^{(n)} | \psi_j^{(n)}\rangle \right). \quad (4n)$$

As was pointed out earlier, the complete detailed prescription of Eqs. (4m) and (4n) for the perturbational iteration of a bound state approximation $|\psi_j^0\rangle$ cannot be obtained within the confines of the *standard* Schrödinger bound-state perturbation approach [4] because that approach makes no attempt to work out the *inhomogeneous* Eq. (4j) or (4k) variant of the stationary-state Schrödinger equation for the exact bound state $|\psi_j\rangle$. Of course having Eq. (4j) *in hand* is *also* absolutely critical for the development of *nonperturbational* “continued fraction” iteration of $\langle \rho_i | \psi_j^0 \rangle$, where $\langle \rho_i | \psi_j^0 \rangle$ must be *nonzero* for every member of the complete

orthogonal basis set $\{\langle\rho_i|\}$. The prescription for that nonperturbational “continued fraction” iteration clearly comes out to be,

$$\left\{ 1 + \left(\langle\rho_i|\psi_j^{(n)}\rangle \right)^{-1} \langle\rho_i| \left[P/(\widehat{H}_0 - E_j^0) \right] \left[\widehat{V} - \left(\langle\psi_j^{(n)}|\widehat{V} + \widehat{H}_0 - E_j^0|\psi_j^{(n)}\rangle / \langle\psi_j^{(n)}|\psi_j^{(n)}\rangle \right) \right] |\psi_j^{(n)}\rangle \right\}, \quad (4o)$$

where, of course, $\langle\rho_i|\psi_j^{(0)}\rangle = \langle\rho_i|\psi_j^0\rangle$, and the approximation $E_j^{(n+1)}$ to the energy eigenvalue is given by Eq. (4n).

For a bound state approximation $|\psi_j^0\rangle$, finding a complete orthogonal basis set $\{\langle\rho_i|\}$ such that every $\langle\rho_i|\psi_j^0\rangle$ is *nonzero* may not be simple because, aside from the ground state, bound states normally have *nodes* (where they of course vanish) in both coordinate and momentum representation. However *if* that bound state approximation $|\psi_j^0\rangle$ is an eigenstate of an “unperturbed” *harmonic oscillator Hamiltonian* \widehat{H}_0 , then one can find a related “harmonic-oscillator coherent false ground-state with false excitations” orthogonal basis $\{\langle\psi(c)_i^0|\}$ such that every $\langle\psi(c)_i^0|\psi_j^0\rangle$ is indeed nonvanishing. Here c is a complex number such that $|c|^2$ is a *transcendental* positive real number, e.g., the natural-logarithm base e or the constant π , and the “false ground state” is the minimum-uncertainty *coherent state* that is characterized by the complex number c , i.e., it is annihilated by one of the harmonic-oscillator *annihilation operators* with c *subtracted from it*. Successive mutually orthogonal states $|\psi(c)_i^0\rangle$ are then generated from this particular *coherent* “false ground state” characterized by c through the repeated action of the *corresponding harmonic-oscillator creation operator* with the *complex conjugate* \bar{c} of c subtracted from it—these are the “false excitations” of the coherent “false ground state”. It turns out that $\langle\psi(c)_i^0|\psi_j^0\rangle$ can’t vanish if $|c|^2$ is a positive transcendental number because it only vanishes when $|c|^2$ is a zero of an appropriate polynomial that has rational coefficients. We note that the *nontranscendental* (i.e., the “algebraic”) real numbers, being a *countable set*, are of measure zero. Furthermore, choosing to use harmonic-oscillator states as bound state approximations is likely a viable proposition, e.g., for a bound state of a three-dimensional system, its approximation by a suitable three-dimensional harmonic oscillator state could probably be made to work out quite well.

Time-dependent Dirac-picture successive approximation methods

It is often the case that the Hamiltonian operator \widehat{H} for a time-dependent Schrödinger equation,

$$i\hbar d(|\psi(t)\rangle)/dt = \widehat{H}|\psi(t)\rangle, \quad (5a)$$

can be written in the form $\widehat{H} = \widehat{H}_0 + \widehat{V}$, where \widehat{H}_0 is *exactly diagonalizable* and $|\psi(t_0)\rangle$ is specified to equal one of the eigenstates $|\psi_0\rangle$ of \widehat{H}_0 . In that case it can be useful to reexpress the time-dependent Schrödinger Eq. (5a) in the *Dirac picture* [5],

$$|\psi(t)\rangle = e^{-i\widehat{H}_0(t-t_0)/\hbar} |\psi_D(t)\rangle, \quad (5b)$$

which yields,

$$i\hbar d(|\psi_D(t)\rangle)/dt = \widehat{V}_D(t) |\psi_D(t)\rangle, \quad (5c)$$

where,

$$\widehat{V}_D(t) \stackrel{\text{def}}{=} e^{i\widehat{H}_0(t-t_0)/\hbar} \widehat{V} e^{-i\widehat{H}_0(t-t_0)/\hbar}, \quad (5d)$$

and $|\psi_D(t_0)\rangle = |\psi_0\rangle$. Through integration, Eq. (5c) can be reexpressed in an *inhomogeneous form* that *incorporates* the eigenstate $|\psi_0\rangle$ of \widehat{H}_0 as the *inhomogeneous term*,

$$|\psi_D(t)\rangle = |\psi_0\rangle - (i/\hbar) \int_{t_0}^t \widehat{V}_D(t') |\psi_D(t')\rangle dt'. \quad (5e)$$

The inhomogeneous Eq. (5e) has the form of our generic Eq. (1a), and therefore is subject to either standard perturbational iteration,

$$|\psi_D^{(n+1)}(t)\rangle = |\psi_0\rangle - (i/\hbar) \int_{t_0}^t \widehat{V}_D(t') |\psi_D^{(n)}(t')\rangle dt', \quad (5f)$$

where of course $|\psi_D^{(0)}(t)\rangle = |\psi_0\rangle$, or, if we can find a complete orthogonal basis set $\{\langle\rho_i|\}$ such that $\langle\rho_i|\psi_0\rangle$ is *never zero*, we can carry out *nonperturbational* “continued-fraction” iteration,

$$\langle\rho_i|\psi_D^{(n+1)}(t)\rangle = \langle\rho_i|\psi_0\rangle / \left[1 + (i/\hbar) \left(\langle\rho_i|\psi_D^{(n)}(t)\rangle \right)^{-1} \int_{t_0}^t \langle\rho_i|\widehat{V}_D(t')|\psi_D^{(n)}(t')\rangle dt' \right], \quad (5g)$$

where of course $\langle \rho_i | \psi_D^{(0)}(t) \rangle = \langle \rho_i | \psi_0 \rangle$.

A prime application of the Dirac-picture Eq. (5e) is to *quantum field theories* [6], where it has invariably so far been pursued by using the standard perturbational iteration scheme of Eq. (5f), no doubt most famously by Dyson to systematically extract the *quintessentially perturbational* Feynman diagrams [6]. It would certainly be interesting if the *nonperturbational* “continued-fraction” iteration scheme of Eq. (5g) could conceivably be applied to quantum field theories.

In quantum-field applications $|\psi_0\rangle$ is a small number of unperturbed boson and fermion particles. Now unperturbed boson systems can be regarded as a massive collection of quantized simple harmonic oscillators, while unperturbed fermion systems can be regarded as an equally massive collection of quantum two-state entities. In the previous section we have pointed out that systems which are initially harmonic oscillators can be made compatible with continued-fraction iteration by using a “coherent false ground state” and related “false excitation” *orthogonal basis* (in quantum field theories perhaps better termed a “coherent false vacuum” and related “false Bose-particle” *orthogonal basis*), wherein quantized oscillator annihilation operators are translated by a complex number, and creation operators by that number’s complex conjugate, which, of course can *also* be described as a simple *real-valued c-number vector translation of the quantum coordinate-momentum operator phase space*. The *reason* that such c-number operator translations simply generate *additional orthogonal bases* is, of course, that c-number translations have *no effect on the crucial commutator algebra of those operators*, i.e., they are *canonical* transformations, indeed *unitary* ones.

Systems which are initially collections of two-state systems would seem in principle even easier to make compatible with “continued-fraction” iteration. In Pauli-matrix language, if the natural basis for the initial two-state system consists of the two eigenstates of $\frac{1}{2}(1 + \sigma_z)$ (which has the two eigenvalues 0 and 1, namely the two natural fermionic-state occupation numbers), then for this particular purpose of “continued fraction” iteration, we can *instead* adopt the two eigenstates of $\frac{1}{2}(1 + \sigma_y)$, for example, since each state of the natural basis indeed has a *nonzero inner product with each one of the states of this adopted basis*. The example just given can be described as a spinor basis rotation of ninety degrees, and other rotation angles ought to achieve the desired result as well. Note that the natural unperturbed-particle basis has here once again been subjected to *a unitary transformation*.

The fact that the continued-fraction iteration scheme *forces* on one a basis that has *no zero-valued inner products* with the members of the natural particle occupation-number basis of the quantum field system’s unperturbed Hamiltonian operator \hat{H}_0 implies that this iteration scheme *will very rapidly indeed* force an *unbounded number* of unperturbed particles into active participation. That is in very sharp contrast with the perturbational iteration scheme: the *intrinsic nature* of Feynman diagrams *immediately reveals* that no more than a *certain maximum number* of unperturbed particles *can ever participate* through a given order of the perturbational iteration. (The only exception to this iron Feynman-diagram rule occurs when individual diagrams *fail by yielding infrared divergences* – whose *cure* is widely agreed to involve *coherent* photon states, *which have no upper bound on the possible number of photons which they describe*). The continued-fraction iteration scheme, contrariwise, *forces on one* coherent states (i.e., “false vacua”) and their related mutually orthogonal “false Bose-particle” brethren that *all* have an unbounded number of unperturbed particles. It *as well* forces on one the fact that *all* the fermionic basis states have a greater than zero probability *to actually be occupied by unperturbed fermions*. Feynman diagrams reveal “virtual particles”, but continued-fraction iteration reveals immense “virtual clouds” *which have no upper bound on the number of unperturbed particles involved*. Landing in the thick of such “virtual clouds” within an iteration or two suggests much better convergence for the continued-fraction scheme than for the perturbational one.

Feynman diagrams can *diverge*. In the continued-fraction scheme, everything that is calculated gets pushed into a *denominator*, which makes actual divergence quite difficult to visualize mathematically. What diverges in the continued-fraction scheme would seem to be *unperturbed-particle participation* rather than the iteration expressions themselves.

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