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Pointed weak energy and quantum state evolution in Pancharatnam–Fubini-Study configuration space

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Abstract

The weak energy for a quantum state evolving relative to its fixed initial state (pointed weak energy) in a Hilbert space of arbitrary dimension is defined and aspects of the classical mechanical, transformational and geometric relationships between this quantity and the motion of the associated quantum state are studied in a two-dimensional configuration space with Pancharatnam (P) phase and Fubini-Study (FS) metric distance as generalized coordinates (PFS configuration space). It is shown that when expressed in these coordinates: (1) the evolution of the quantum state is described by an equation of motion for an associated correlation amplitude (pointed correlation amplitude) in which the dynamics are induced by the interaction of the pointed weak energy with this correlation amplitude; (2) the pointed weak energy defines a 1-form with the transformational properties of a $U(1)$ gauge potential (pointed weak energy gauge potential) which produces infinitesimal changes in the pointed correlation amplitude via its interaction with the amplitude; (3) the pointed correlation amplitude is defined by an exponential function of a line integral of the pointed weak energy gauge potential; (4) pointed weak energy gauge transformations exist that are equivalent to local $U(1)$ gauge transformations of quantum states and—when examined within the context of the pointed probability current and pointed weak energy stationary action principles—offer an interpretation of gauge invariance analogous to that found in classical mechanics; and (5) integral invariants exist which relate line integrals of the weak energy gauge potential to geometric phase and the Aharonov–Anandan connection 1-form in the associated Hilbert space. States which irreversibly decay and Grover's quantum search algorithm serve as simple illustrations of the theory.

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1. Introduction

A complex-valued energy which is associated with a collection of quantum states evolving in Hilbert space has recently been defined and studied from a theoretical perspective [1]. Because the mathematical form of this quantity is the same as that used by Aharonov *et al* [2–4] to define the 'weak value' of a quantum mechanical observable, this complex-valued energy is analogously called the *weak energy* for a quantum state system. It was shown in [1] that the weak energy associated with a set of contemporaneously evolving states in a Hilbert space can be expressed in terms of the Pancharatnam (*P*) phases and the Fubini-Study (*FS*) metric distances separating them. In this *PFS* representation, the weak energy satisfies the formalism of the concomitant Euler–Lagrange equations and provides for a weak energy stationary action principle. This principle is analogous to the well known *Hamilton's principle* of classical mechanics and describes the paths in Hilbert space followed by quantum states as they evolve between their initial and final end point configurations.

The purpose of this paper is to examine in the PFS representation certain classical mechanical, transformational and geometric aspects that are associated with weak energy and its relationship to the motion of a quantum state evolving relative to its fixed initial state in a Hilbert space of arbitrary dimension. Although several new and special case ancillary results are discussed in the subsequent development—when briefly and collectively stated—the main new results reported in this paper are that, in a PFS representation which is referenced to a fixed initial quantum state: (1) the evolution of the quantum state is described by an equation of motion for an associated complex-valued correlation amplitude which is functionally dependent upon a P phase and an FS distance and for which the dynamics are induced by the interaction of the weak energy with the correlation amplitude; (2) the weak energy satisfies the Euler–Lagrange equations for generalized PFS coordinates and defines a 1-form with the transformational properties of a $U(1)$ gauge potential which produces infinitesimal changes in the correlation amplitude via the interaction between this potential and the correlation amplitude; (3) the associated correlation amplitude is defined by an exponential function of a line integral of this gauge potential; (4) weak energy gauge transformations can be defined which are equivalent to local $U(1)$ gauge transformations of quantum states and—when examined within the context of the probability current and weak energy stationary action principles developed below—offer an interpretation of gauge invariance analogous to that found in classical mechanics; and (5) integral invariants exist which relate line integrals of the weak energy gauge potential to geometric phase and the Aharonov–Anandan connection 1-form in the associated Hilbert space.

The remainder of this paper is organized as follows: in the next section, PFS configuration space is formally described in terms of a pointed map from a subset of states in Hilbert space into the real plane; PFS configuration space images under this map of evolutionary paths of states in Hilbert space are discussed; and *pointed weak energy* and the *PFS 1-form* are defined. The functional form and the equation of motion in the PFS representation for the state correlation amplitude relative to its initial state, i.e. the *pointed correlation amplitude*, are both obtained in section 3. There it is shown that this amplitude is defined by an exponential function of an associated line integral of the PFS 1-form and that its time rate of change is produced by a pointed weak energy-correlation amplitude interaction. It is also demonstrated in this section that the partial derivatives of the pointed correlation amplitude with respect to the generalized PFS coordinates act as generalized PFS momentum component operators. This property allows the equation of motion for the pointed correlation amplitude to be written in a compact vector form that is expressed in terms of PFS velocity and gradient vectors and provides for a definition of the pointed weak energy operator in terms of these quantities.

In the next section, gauge transformations of the pointed weak energy are introduced and they are shown to be equivalent to local $U(1)$ gauge transformations of quantum states when the arguments of the phase factors are differentiable functions of the PFS coordinates of the states. The pointed weak energy gauge potential is also identified and its interaction with the pointed correlation amplitude is shown to induce infinitesimal changes in the correlation amplitude. The *pointed probability current* is defined in section 5 and used to establish an associated *pointed probability current stationary action principle*. Although it is a special case of the weak energy stationary action principle [1]—for the sake of completeness—the *pointed weak energy stationary action principle* is also stated since gauge invariance is discussed in this section within the context of both the pointed weak energy and pointed probability current stationary action principles. It is also noted there that the form invariance of the equation of motion for the correlation amplitude, as well as that describing its infinitesimal change, is possible only because of the gauge transformation properties of the pointed weak energy and the gauge potential. In section 6, the gauge invariance of the pointed weak energy action difference is employed to obtain a first order relative integral invariant in PFS configuration space that can be related to special pairs of quantum state evolutionary paths in Hilbert space. In addition, associated paths and line integrals provide two-dimensional descriptions of the phases of quantum states evolving in the Hilbert space and establish interesting relationships between the pointed weak energy gauge potential, geometric phase and the Aharonov–Anandan connection 1-form. Irreversible decay processes and Grover's quantum search algorithm serve to illustrate aspects of the theory in section 7. Concluding remarks comprise the final section of this paper.

2. PFS configuration space, pointed weak energy and the PFS 1-form

Let $|\psi_0\rangle$ be a distinguished state (or point) in the Hilbert space $\mathcal{H}$ with projective space $\mathcal{P}$ consisting of all the rays of $\mathcal{H}$ (recall that a ray is an equivalence class $[\psi]$ of states $|\psi\rangle$ in $\mathcal{H}$ which differ only in phase) and with induced projection map $\Pi : \mathcal{H} \to \mathcal{P}$ such that $|\psi\rangle \overset{\Pi}{\longmapsto} [\psi]$. Also, let $\mathcal{H}_{\sim\perp}$ be the subset of states of $\mathcal{H}$ given by $\mathcal{H}_{\sim\perp} = \{|\psi\rangle \in \mathcal{H} : \langle\psi|\psi_0\rangle \neq 0\}$ and define the pointed map $\Psi_0 : \mathcal{H}_{\sim\perp} \to \mathcal{R} \times \mathcal{R}$ by

$$\Psi_0(|\psi\rangle) \equiv \left(\arg \frac{\langle\psi|\psi_0\rangle}{|\langle\psi|\psi_0\rangle|}, 2\sqrt{1 - |\langle\psi|\psi_0\rangle|^2}\right) = (\chi, s),$$

where $\mathcal{R}$ is the set of real numbers (Ψ_0 is 'pointed' in the sense that the distinguished state is mapped to $(0, 0)$). Here $\chi \in [0, 2\pi)$ is the Pancharatnam phase [5] defined by

$$\mathrm{e}^{\mathrm{i}\chi} \equiv \frac{\langle\psi|\psi_0\rangle}{|\langle\psi|\psi_0\rangle|}. \tag{1}$$

This quantity is the phase difference between $|\psi_0\rangle$ and $|\phi\rangle$, where $|\phi\rangle$ is the state contained in $[\psi_0]$ obtained by parallel transporting $|\psi\rangle$ along the unique path in $\mathcal{H}$ which is the pre-image under Π of the shortest geodesic joining $[\psi]$ and $[\psi_0]$ in $\mathcal{P}$ [6]. The quantity s is the generalized Fubini-Study metric distance s separating $[\psi]$ and $[\psi_0]$ in $\mathcal{P}$ defined by [7 ,8]

$$s^2 \equiv 4(1 - |\langle\psi|\psi_0\rangle|^2). \tag{2}$$

The restriction of the domain of Ψ_0 to the set $\mathcal{H}_{\sim\perp}$ avoids division by zero in equation (1) and naturally confines values of s to the real interval $[0, 2)$. Thus, the *PFS configuration space* $\mathcal{B}$ associated with any distinguished state $|\psi_0\rangle$ is the image set $\mathcal{B} \equiv \mathrm{Im}\,\Psi_0 = [0, 2\pi) \times [0, 2) \subset \mathcal{R} \times \mathcal{R}$. Note that the map Ψ_0 provides an equivalence classification of the states in $\mathcal{H}_{\sim\perp}$. More specifically, the states $|\psi\rangle$ and $|\psi'\rangle$ are equivalent under Ψ_0, i.e. $|\psi\rangle \sim |\psi'\rangle$, when $\Psi_0(|\psi\rangle) = \Psi_0(|\psi'\rangle)$.

Consider now the case for which $|\psi\rangle = |\psi(t)\rangle$ with $|\psi_0\rangle = |\psi(0)\rangle$ and such that the evolution of $|\psi(t)\rangle$ over the time interval $[0, \tau]$ occurs continuously and entirely within $\mathcal{H}_{\sim\perp}$, i.e. $|\psi(t)\rangle \in \mathcal{H}_{\sim\perp}$ for every $t \in [0, \tau]$. In particular, let the map $\alpha : [0, \tau] \to \mathcal{H}_{\sim\perp}$ define such an evolutionary path with $|\psi(t)\rangle = \alpha(t)$. Then the composition of maps $\gamma \equiv \Psi_0 \circ \alpha$ is the curve which describes this evolution in $\mathcal{B}$ and has $\gamma(0) = (\chi(0), s(0)) = (0, 0)$ as its first point and $\gamma(\tau) = (\chi(\tau), s(\tau))$ as its last point. The curve γ is *simple* if γ is an injective map and is *closed* if $\gamma(0) = \gamma(\tau)$. The closed curve γ is simple if the restriction of γ to the domain $(0, \tau)$ is injective. An evolutionary path in $\mathcal{H}$ over $[0, \tau]$ for which $|\psi(t)\rangle \in \mathcal{H}_{\sim\perp}, t \in [0, \tau]$, and for which γ is a smooth curve is said to be *proper* and the curve γ is the associated *proper evolution in* $\mathcal{B}$.

Let the normalized quantum state $|\psi(t)\rangle$ with initial state $|\psi(0)\rangle$ follow a proper evolutionary path in $\mathcal{H}$. The *pointed weak energy* W_0 associated with this state at time t relative to its initial state is the complex-valued quantity defined by

$$W_0(t) \equiv \frac{\langle\psi(t)|\widehat{H}|\psi(0)\rangle}{\langle\psi(t)|\psi(0)\rangle} = \operatorname{Re} W_0(t) + \mathrm{i} \operatorname{Im} W_0(t), \tag{3}$$

where

$$\mathrm{i}\hbar \frac{\mathrm{d}|\psi(t)\rangle}{\mathrm{d}t} = \widehat{H}|\psi(t)\rangle.$$

Clearly, $W_0(0)$ is the mean energy at $t = 0$. It is easily determined from equations (1) and (2) that

$$\operatorname{Re} W_0(t) = \hbar\left(\frac{\mathrm{d}\chi(t)}{\mathrm{d}t}\right) \equiv \hbar\dot{\chi}(t)$$

and

$$\operatorname{Im} W_0(t) = \hbar\left\{\frac{s(t)}{4 - s^2(t)}\right\}\left(\frac{\mathrm{d}s(t)}{\mathrm{d}t}\right) \equiv \hbar\left\{\frac{s(t)}{4 - s^2(t)}\right\}\dot{s}(t).$$

Consequently, the pointed weak energy of equation (3) assumes the following form in the PFS representation:

$$\mathcal{L}_0(s(t); \dot{\chi}(t), \dot{s}(t)) \equiv \hbar\dot{\chi}(t) + \mathrm{i}\hbar\left\{\frac{s(t)}{4 - s^2(t)}\right\}\dot{s}(t). \tag{4}$$

Using equation (4) it is easily verified that the Euler–Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\mathcal{L}_0}{\partial\dot{y}}\right) = \frac{\partial\mathcal{L}_0}{\partial y}, \tag{5}$$

for the pointed weak energy are satisfied for the generalized coordinates $y = \chi, s$. Thus, the associated generalized momenta are defined by

$$p_\chi = \frac{\partial\mathcal{L}_0}{\partial\dot{\chi}} = \hbar, \tag{6}$$

and

$$p_s = \frac{\partial\mathcal{L}_0}{\partial\dot{s}} = \mathrm{i}\hbar\frac{s}{4 - s^2}, \tag{7}$$

where p_χ and p_s are the Pancharatnam and the Fubini-Study momenta, respectively. Substituting these last two identities into equation (4) provides the following useful expression for the pointed weak energy:

$$\mathcal{L}_0 = p_\chi\dot{\chi} + p_s\dot{s}. \tag{8}$$

Using this, the *PFS 1-form* ω_0 is defined as

$$\omega_0 \equiv \hbar^{-1}\mathcal{L}_0\,\mathrm{d}t = \hbar^{-1}(p_\chi\,\mathrm{d}\chi + p_s\,\mathrm{d}s).$$

Observe that ω_0 is an exact 1-form because there exists a continuous function $f(\chi, s) = \chi - \frac{\mathrm{i}}{2}\ln\left(\frac{4-s^2}{4}\right)$ with continuous partial derivatives with respect to χ and s such that $\omega_0 = \mathrm{d}f$. It follows that for any smooth curve γ in $\mathcal{B}$ which connects (0, 0) to any other point (χ', s'),

$$\int_\gamma \omega_0 = f(\chi', s'), \tag{9}$$

i.e. *the value of* $\int_\gamma \omega_0$ *is independent of the path taken between* (0, 0) *and* (χ', s') in $\mathcal{B}$.

3. The pointed correlation amplitude and its equation of motion

The PFS representation $\varphi(\chi, s)$ for the correlation amplitude $\langle\psi(t)|\psi(0)\rangle$, i.e. the *pointed correlation amplitude*, can be obtained from the general time translation equation for correlation amplitudes given by [1]

$$\langle\psi_j(t_1)|\psi_k(t_1)\rangle = \exp\left(\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t_1}\mathcal{L}(s_{j,k};\,\dot{\chi}_{j,k},\dot{s}_{j,k})\,\mathrm{d}t\right)\langle\psi_j(t_0)|\psi_k(t_0)\rangle$$

by assigning $|\psi_j(t_1)\rangle = |\psi(t)\rangle, |\psi_k(t_1)\rangle = |\psi(0)\rangle, |\psi_j(t_0)\rangle = |\psi_k(t_0)\rangle$, and by setting the integration limits to be $t_1 = t$ and $t_0 = 0$. In this case, the integrand in the exponential is the pointed weak energy so that the last equation becomes

$$\langle\psi(t)|\psi(0)\rangle = \exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t \mathcal{L}_0(s;\,\dot{\chi},\dot{s})\,\mathrm{d}t'\right) \equiv \varphi(\chi, s). \tag{10}$$

If the evolution of $|\psi\rangle$ is proper over the time interval $[0, t]$ and the curve γ is the associated proper evolution in $\mathcal{B}$, then the last equation may also be written as

$$\varphi(\chi, s) \equiv \exp\left(\mathrm{i}\int_\gamma \omega_0\right). \tag{11}$$

The form of this equation demonstrates that for proper evolutionary paths the pointed correlation amplitude is not only defined by the evaluation of the PFS 1-form on the curve γ in $\mathcal{B}$, but also shows—because of path independence—that in general the value of φ is the same for all paths in $\mathcal{B}$ with the same last point.

Since ω_0 is exact, the evaluation of this line integral is trivial and depends only upon the last point (χ, s) of γ. Application of equation (9) to equation (11) quickly provides the simple result

$$\varphi(\chi, s) = \tfrac{1}{2}\sqrt{4 - s^2}\,\mathrm{e}^{\mathrm{i}\chi}. \tag{12}$$

Straightforward time differentiation of φ yields

$$\dot{\varphi} = \frac{\mathrm{i}}{\hbar}\mathcal{L}_0\varphi \tag{13}$$

as its equation of motion. It is clear from this that the interaction $\mathcal{L}_0\varphi$ between the pointed weak energy and the pointed correlation amplitude is responsible for producing the pointed correlation amplitude's time rate of change.

The function φ exhibits an interesting property that enables equation (13) to be written in a compact vector form. In particular, it is easily verified from equation (12), (6) and (7) that

$$\frac{\hbar}{\mathrm{i}}\frac{\partial\varphi}{\partial\chi} = p_\chi\varphi \qquad \text{and} \qquad \frac{\hbar}{\mathrm{i}}\frac{\partial\varphi}{\partial s} = p_s\varphi,$$

i.e. *the partial derivatives of* φ *with respect to* χ *or* s *behave as generalized PFS momentum component operators*. As a check of the validity of these identities, note that their application to the right-hand side of equation (13) yields the required following form for the total time derivative of φ:

$$\dot{\varphi} = \left(\frac{\partial \varphi}{\partial \chi}\right)\dot{\chi} + \left(\frac{\partial \varphi}{\partial s}\right)\dot{s}.$$

If $\widehat{e}_\chi$ and $\widehat{e}_s$ are orthogonal unit vectors in $\mathcal{B}$ at the origin and along the χ and s axes, respectively, then PFS velocity and gradient vectors can be defined as $\overrightarrow{v} \equiv \dot{\chi}\widehat{e}_\chi + \dot{s}\widehat{e}_s$ and $\overrightarrow{\nabla} \equiv \widehat{e}_\chi \frac{\partial}{\partial \chi} + \widehat{e}_s \frac{\partial}{\partial s}$, respectively. Using these definitions in the last equation provides the following vector form for the equation of motion for φ:

$$\dot{\varphi} = \overrightarrow{v} \cdot \overrightarrow{\nabla}\varphi.$$

Comparison of the right-hand side of the last equation with that of equation (13) also reveals that

$$\frac{\hbar}{\mathrm{i}}\overrightarrow{v} \cdot \overrightarrow{\nabla}\varphi = \mathcal{L}_0\varphi,$$

i.e. *the product* $\frac{\hbar}{\mathrm{i}}\overrightarrow{v} \cdot \overrightarrow{\nabla}$ *behaves as a pointed weak energy operator when it acts upon* φ.

4. Pointed weak energy gauge transformations and the pointed weak energy gauge potential

Consider the pointed weak energy transformation given by

$$\mathcal{L}_0^\theta(\chi^\theta, s^\theta; \dot{\chi}^\theta, \dot{s}^\theta) = \mathcal{L}_0(s; \dot{\chi}, \dot{s}) - \hbar\dot{\theta}(\chi, s), \tag{14}$$

where $\theta = \theta(\chi, s)$ is a dimensionless function with continuous derivatives. Since transformations of this form with $\mathcal{L}_0$ replaced by a Lagrangian energy function are referred to as gauge transformations in the classical mechanics literature (e.g., Rund [9]), then, by analogy, equation (14) will be called a *pointed weak energy gauge transformation*. The effect of this transformation upon φ and $|\psi(t)\rangle$ can be ascertained from equation (10) by replacing the integrand in the exponential with equation (14). It is then found that

$$\varphi^\theta = \exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t \mathcal{L}_0^\theta \,\mathrm{d}t'\right) = \exp\left(\frac{\mathrm{i}}{\hbar}\int_0^t \mathcal{L}_0 \,\mathrm{d}t'\right)\exp\left(-\mathrm{i}[\theta]_0^t\right) = \varphi\exp(-\mathrm{i}(\theta_t - \theta_0)),$$

(the functional dependences are omitted for the sake of notational brevity), where $\theta_t \equiv \theta(\chi(t), s(t)) = \theta$. This clearly implies that $|\psi(t)\rangle$ consequently transforms into $\mathrm{e}^{\mathrm{i}\theta_t}|\psi(t)\rangle$ (with $\mathcal{L}_0^\theta$ as its associated pointed weak energy). Since the converse of this is also true, it can be concluded that a pointed weak energy gauge transformation is equivalent to a local $U(1)$ gauge transformation of the state $|\psi(t)\rangle$ in which the argument of the transformation is an arbitrary differentiable function that has its positional dependence specified in terms of the generalized PFS coordinates of the state at time t, i.e. by $\Psi_0(|\psi(t)\rangle)$.

Note from equations (1) and (2) that the state transformation $|\psi(t)\rangle \to \mathrm{e}^{\mathrm{i}\theta_t}|\psi(t)\rangle$ yields $\chi \to \chi' = \chi - (\theta_t - \theta_0)$ and $s \to s' = s$ as its PFS coordinate transformation. Under this transformation, the image of the evolutionary path for $\mathrm{e}^{\mathrm{i}\theta_t}|\psi(t)\rangle$ in $\mathcal{B}$ differs from that for $|\psi(t)\rangle$ in $\mathcal{B}$ and in general does not have (0, 0) as its first point. However—provided that θ is differentiable—it is easy to see using equation (8) and

$$\dot{\theta} = \frac{\partial \theta}{\partial \chi}\dot{\chi} + \frac{\partial \theta}{\partial s}\dot{s}$$

that the pointed weak energy gauge transformation of equation (14) defines the following *canonical pointed weak energy gauge transformation* of the generalized PFS coordinates and momenta:

$$\chi^\theta = \chi, \qquad s^\theta = s, \qquad p_\chi^\theta = p_\chi - \hbar \frac{\partial \theta}{\partial \chi} \qquad \text{and} \qquad p_s^\theta = p_s - \hbar \frac{\partial \theta}{\partial s}. \tag{15}$$

Although the PFS momenta are changed by this transformation, the PFS coordinates are not. Thus, both $|\psi(t)\rangle$ and $e^{i\theta_t}|\psi(t)\rangle$ describe the same evolutionary path in $\mathcal{B}$ with $(0, 0)$ as its first point. Furthermore, since $\chi^\theta = \chi \Rightarrow \dot{\chi}^\theta = \dot{\chi}$ and $s^\theta = s \Rightarrow \dot{s}^\theta = \dot{s}$, then both states also evolve in $\mathcal{B}$ at the same rate. The replacement pair

$$\varphi \to \varphi^\theta \qquad \text{and} \qquad \mathcal{L}_0 \to \mathcal{L}_0^\theta$$

is termed a *general canonical pointed weak energy gauge transformation*.

It is interesting to observe that $\mathcal{L}_0$ defines $\omega_0 = \hbar^{-1}\mathcal{L}_0\, dt$ as a $U(1)$ gauge potential called the *pointed weak energy gauge potential*. That ω_0 can be identified as a gauge potential is a direct consequence of the fact that under the gauge transformation $|\psi\rangle \to e^{i\theta_t}|\psi\rangle$, ω_0 obeys the transformation rule

$$\omega_0^\theta = \omega_0 + d(i \ln g) = \omega_0 - d\theta_t, \tag{16}$$

where $\omega_0^\theta \equiv \hbar^{-1}\mathcal{L}_0^\theta\, dt$ and $g \equiv e^{i\theta_t} \in U(1)$. To see this, simply write $\omega_0^\theta = \hbar^{-1}\big(p_\chi^\theta\, d\chi + p_s^\theta\, ds\big) = \hbar^{-1}\big(p_\chi - \hbar\frac{\partial\theta_t}{\partial\chi}\big)\, d\chi + \hbar^{-1}\big(p_s - \hbar\frac{\partial\theta_t}{\partial s}\big)\, ds = \hbar^{-1}(p_\chi\, d\chi + p_s\, ds) - \big(\frac{\partial\theta_t}{\partial\chi}\, d\chi + \frac{\partial\theta_t}{\partial s}\, ds\big) = \omega_0 - d\theta_t$. The pair of replacements

$$\varphi \to \varphi^\theta \qquad \text{and} \qquad \omega_0 \to \omega_0^\theta$$

is called a *general pointed weak energy gauge potential transformation*.

It follows from equation (11) that φ can now also be considered to be defined by an exponential function of a line integral of the pointed weak energy gauge potential. It is readily determined from equation (13) that

$$d\varphi = \frac{i}{\hbar}\mathcal{L}_0 \varphi\, dt = i\omega_0\varphi \tag{17}$$

(upon integration, this equation yields, as it must, equation (11)). It can be concluded from this that in the PFS representation infinitesimal changes of the pointed correlation amplitude are induced by the interaction $\omega_0\varphi$ between the pointed weak energy gauge potential and the pointed correlation amplitude.

5. Stationary action principles and gauge invariance

Equation (12) leads to a new stationary action principle. In particular, for a proper evolution in $\mathcal{H}$, the associated *pointed probability current* $\mathcal{C}$ is defined as

$$\mathcal{C}(s, \dot{s}) \equiv \frac{d\,\Pr(s)}{dt} = -\frac{1}{2} s\dot{s},$$

where $\Pr(s)$ is the pointed correlation probability given by

$$\Pr(s) \equiv \varphi^*(\chi, s)\varphi(\chi, s) = \tfrac{1}{4}(4 - s^2). \tag{18}$$

This quantity is the probability that the system is in state $|\psi(0)\rangle$ at time $t \geqslant 0$. Note that the right-hand side of equation (12) can also be expressed as $\sqrt{\Pr(s)}\, e^{i\chi}$.

It is readily verified that $\mathcal{C}$ satisfies the Euler–Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial\mathcal{C}}{\partial\dot{s}}\right) = \frac{\partial\mathcal{C}}{\partial s}.$$

Consequently, the action

$$J_0 \equiv \int_0^\tau \mathcal{C}(s(t), \dot{s}(t))\, dt$$

that is associated with the proper evolution of a quantum state relative to its initial state in $\mathcal{H}$ during some time interval $[0, \tau]$ is stationary for fixed end points. This is formalized as the *pointed probability current stationary action principle* which states that *the actual proper evolutionary path followed in $\mathcal{H}$ by the state $|\psi(t)\rangle$ between the end points $|\psi(0)\rangle$ and $|\psi(\tau)\rangle$ for times $\tau > 0$ is such that the action J_0 is stationary for all variations in s and time which vanish at the end points*.

Since the Euler–Lagrange equations (5) are satisfied for the pointed weak energy, then the action I_0 defined by the canonical integral

$$I_0 \equiv \int_0^\tau \mathcal{L}_0(s(t); \dot{\chi}(t), \dot{s}(t))\, dt$$

that is associated with the proper evolution of a quantum state $|\psi(t)\rangle$ in $\mathcal{H}$ relative to its initial state $|\psi(0)\rangle$ during a time interval $[0, \tau]$ is stationary whenever the end points at $t = 0$ and $t = \tau$ are fixed. This is formalized as the *pointed weak energy stationary action principle* which states that *the actual proper evolutionary path followed in $\mathcal{H}$ by the state $|\psi(t)\rangle$ between the end points $|\psi(0)\rangle$ and $|\psi(\tau)\rangle$ for times $\tau > 0$ is such that the action I_0 is stationary for all variations in χ, s, and time which vanish at the end points*. Although this principle is a special case of the weak energy stationary action principle [1], as noted above—it is stated here because of its relevance to the subsequent discussion concerning gauge invariance. For additional details about associated momentum and energy conservation laws, the reader is referred to [1].

An examination of the relationships between the gauge transformation of equation (14) and the pointed weak energy and pointed probability current stationary action principles is important for identifying state evolutionary properties that are associated with gauge invariance. In particular, consider the proper evolutionary paths for $|\psi(t)\rangle$ and $e^{i\theta_t}|\psi(t)\rangle$ in $\mathcal{H}$ during $[0, \tau]$. Since

$$\int_0^\tau \mathcal{L}_0^\theta\, dt = \int_0^\tau \mathcal{L}_0\, dt - \hbar \int_0^\tau \dot{\theta}\, dt = \int_0^\tau \mathcal{L}_0\, dt - \hbar[\theta]_0^\tau,$$

then performing path variation by applying the first variation δ to both sides of the last equation while keeping the end points fixed yields

$$\delta \int_0^\tau \mathcal{L}_0^\theta\, dt = \delta \int_0^\tau \mathcal{L}_0\, dt.$$

Thus, the variational equation $\delta \int_0^\tau \mathcal{L}_0\, dt = 0$ is equivalent to $\delta \int_0^\tau \mathcal{L}_0^\theta\, dt = 0$ and the pointed weak energy stationary action principle remains true under pointed weak energy gauge transformations of the form given by equation (14). This principle is therefore gauge invariant in the sense that its validity is not affected when applied to a properly evolving gauge transformed state $e^{i\theta_t}|\psi(t)\rangle$—provided that the integrand of the action I_0 is replaced with $\mathcal{L}_0^\theta$ and the end point states $|\psi(0)\rangle$ and $|\psi(\tau)\rangle$ are multiplied by the appropriate phase factors $e^{i\theta_0}$ and $e^{i\theta_\tau}$, respectively. In a similar sense, the pointed probability current stationary action principle is also invariant under pointed weak energy gauge transformations because the current $\mathcal{C}$ and, consequently, the action J_0 are unchanged under such transformations. This follows from the facts that equation (14) is equivalent to a local $U(1)$ gauge transformation and that $U(1)$ is an isometry group for $\mathcal{P}$ when distance is determined by the Fubini-Study metric so that s is a gauge invariant quantity.

This type of *pointed weak energy gauge invariance* is similar to the gauge invariance found in classical mechanics where the variation of the action appearing in Hamilton's principle remains unchanged when the total time derivative of a function of the system coordinates is subtracted from the associated Lagrangian function. Here, although $\mathcal{L}_0^\theta$ is in general not equal in value to $\mathcal{L}_0$, the fact that $\delta\int_0^\tau \mathcal{L}_0^\theta\,\mathrm{d}t = 0$ implies that—not only does $\mathcal{L}_0^\theta$ describe the evolution of a quantum state just as effectively as $\mathcal{L}_0$ (recall that since $\Pi(|\psi(t)\rangle) = \Pi(\mathrm{e}^{\mathrm{i}\theta_t}|\psi(t)\rangle)$, then both distinct evolutionary paths in $\mathcal{H}$ have the same image in the 'physical' projective space $\mathcal{P}$)—but also that (as will be demonstrated in the next paragraph) $\mathcal{L}_0^\theta$ must satisfy the transformed Euler–Lagrange equations. Also, from transformation (15) and the associated discussion in the last section, it can be concluded that both the image and rate of change in $\mathcal{B}$ of a proper evolutionary path for $|\psi(t)\rangle$ in $\mathcal{H}$ over a time interval $[0, \tau]$ remains invariant under transformation (15) when $|\psi(t)\rangle \to \mathrm{e}^{\mathrm{i}\theta_t}|\psi(t)\rangle$ and θ_t is a differentiable function of the PFS coordinates for state $|\psi(t)\rangle$. This result is intuitively pleasing because now it is not only true that $\Pi(|\psi(t)\rangle) = \Pi(\mathrm{e}^{\mathrm{i}\theta_t}|\psi(t)\rangle)$ in $\mathcal{P}$, but it is also true (for appropriate θ_t) that $\Psi_0(|\psi(t)\rangle) = \Psi_0(\mathrm{e}^{\mathrm{i}\theta_t}|\psi(t)\rangle)$ in $\mathcal{B}$.

By writing $\mathcal{L}_0^\theta = p_\chi^\theta\dot{\chi}^\theta + p_s^\theta\dot{s}^\theta$ and using the facts that $\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\theta}{\partial\chi}\right) = \frac{\partial\dot{\theta}}{\partial\chi}$ and $\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\theta}{\partial s}\right) = \frac{\partial\dot{\theta}}{\partial s}$, it is readily verified (as required above by the condition $\delta\int_0^\tau \mathcal{L}_0^\theta\,\mathrm{d}t = 0$) that $\mathcal{L}_0^\theta$ indeed satisfies the associated transformed Euler–Lagrange equations. Consequently, equation (5) remains valid after performing the replacements $y \to y^\theta$, $\frac{\partial\mathcal{L}_0}{\partial\dot{y}} = p_y \to p_y^\theta$, and $\mathcal{L}_0 \to \mathcal{L}_0^\theta$ so that the forms of the Euler–Lagrange equations are preserved under canonical pointed weak energy gauge transformations, i.e.

$$\frac{\mathrm{d}p_y^\theta}{\mathrm{d}t} = \frac{\partial\mathcal{L}_0^\theta}{\partial y^\theta}, \qquad y = \chi, s.$$

It is also of interest to determine the equation of motion for the gauge transformed pointed correlation amplitude $\varphi^\theta \equiv \varphi\,\mathrm{e}^{-\mathrm{i}(\theta_t-\theta_0)}$. After taking the time derivative of each side of this equality and applying the transformations of equation (15), it is found that

$$\dot{\varphi}^\theta = \frac{\mathrm{i}}{\hbar}\mathcal{L}_0^\theta\varphi^\theta = \frac{\mathrm{i}}{\hbar}\left[p_\chi^\theta\dot{\chi}^\theta + p_s^\theta\dot{s}^\theta\right]\varphi^\theta, \tag{19}$$

so that the form of equation (13) is preserved under application of the general canonical pointed weak energy gauge transformation. Thus, it can be concluded that if φ is a solution to equation (13) with $\mathcal{L}_0$ as the pointed weak energy, then φ^θ is the corresponding solution in the gauge with $\mathcal{L}_0^\theta$ as the pointed weak energy so that—in this regard—equation (13) is equivalent to equation (19). Also observe that since $\mathrm{d}\varphi^\theta = \mathrm{e}^{-\mathrm{i}(\theta_t-\theta_0)}\,\mathrm{d}\varphi - \mathrm{i}\mathrm{e}^{-\mathrm{i}(\theta_t-\theta_0)}\varphi\,\mathrm{d}\theta_t = \mathrm{i}\mathrm{e}^{-\mathrm{i}(\theta_t-\theta_0)}\omega_0\varphi - \mathrm{i}\mathrm{e}^{-\mathrm{i}(\theta_t-\theta_0)}\varphi\,\mathrm{d}\theta_t = \mathrm{i}\omega_0^\theta\varphi^{t\theta}$, then the form of equation (17) is preserved under application of the general pointed weak energy gauge potential transformation. It can therefore be concluded that if φ is a solution to equation (17) with ω_0 as the pointed weak energy gauge potential, then φ^θ is the corresponding solution in the gauge with ω_0^θ as the pointed weak energy gauge potential and equation (17) is equivalent to the equation $\mathrm{d}\varphi^\theta = \mathrm{i}\omega_0^\theta\varphi^\theta$. Note that these equivalences hold true only because of the gauge transformation properties of $\mathcal{L}_0$ and ω_0 and—for the case of equation (17)—specifically because ω_0 is a gauge potential.

6. Integral invariants and geometric phase

Consider the two states $|\psi(t)\rangle$ and $|\psi'(t)\rangle$ evolving along proper evolutionary paths in $\mathcal{H}$ over a time interval $[0, \tau]$ such that $|\psi(0)\rangle = |\psi'(0)\rangle$ and $|\psi(\tau)\rangle \sim |\psi'(\tau)\rangle$. Call such paths *last point equivalent paths* and let γ and γ' be the simple curves with identical first and last points which describe these evolutionary paths for $|\psi(t)\rangle$ and $|\psi'(t)\rangle$ in $\mathcal{B}$, respectively. Also, let $\mathcal{L}_0 \equiv \mathcal{L}_0(s; \dot{\chi}, \dot{s})$ and $\mathcal{L}_0' \equiv \mathcal{L}_0(s'; \dot{\chi}', \dot{s}')$ be the respective pointed weak energies. If both

$\mathcal{L}_0$ and $\mathcal{L}'_0$ undergo the same pointed weak energy gauge transformation, then the associated action differences are

$$\int_0^\tau \mathcal{L}_0^\theta\,\mathrm{d}t - \int_0^\tau \mathcal{L}_0\,\mathrm{d}t = -\hbar[\theta(\chi, s)]_0^\tau \equiv -\hbar[\theta]_0^\tau$$

and

$$\int_0^\tau \mathcal{L}_0'^\theta\,\mathrm{d}t - \int_0^\tau \mathcal{L}'_0\,\mathrm{d}t = -\hbar[\theta(\chi', s')]_0^\tau \equiv -\hbar[\theta']_0^\tau.$$

However, $\theta_0 = \theta'_0$ and since $|\psi(\tau)\rangle \sim |\psi'(\tau)\rangle$, then it is also true that $\theta_\tau = \theta'_\tau$ in which case $\hbar[\theta]_0^\tau = \hbar[\theta']_0^\tau$. Thus, the action differences are gauge invariant because

$$\int_0^\tau \mathcal{L}_0^\theta\,\mathrm{d}t - \int_0^\tau \mathcal{L}_0\,\mathrm{d}t = -\hbar[\theta]_0^\tau = -\hbar[\theta']_0^\tau = \int_0^\tau \mathcal{L}_0'^\theta\,\mathrm{d}t - \int_0^\tau \mathcal{L}'_0\,\mathrm{d}t.$$

Upon rearrangement of terms, this expression becomes

$$\int_0^\tau \mathcal{L}_0^\theta\,\mathrm{d}t - \int_0^\tau \mathcal{L}_0'^\theta\,\mathrm{d}t = \int_0^\tau \mathcal{L}_0\,\mathrm{d}t - \int_0^\tau \mathcal{L}'_0\,\mathrm{d}t. \tag{20}$$

Observe that $\hbar^{-1}\mathcal{L}_0^\theta\,\mathrm{d}t$ and $\hbar^{-1}\mathcal{L}_0\,\mathrm{d}t$ are equivalent to the PFS 1-forms ω_0^θ and ω_0 defined by $\omega_0^\theta \equiv \hbar^{-1}\left(p_\chi^\theta\,\mathrm{d}\chi^\theta + p_s^\theta\,\mathrm{d}s^\theta\right) = \hbar^{-1}\left(p_\chi^\theta\,\mathrm{d}\chi + p_s^\theta\,\mathrm{d}s\right)$ and $\omega_0 \equiv \hbar^{-1}(p_\chi\,\mathrm{d}\chi + p_s\,\mathrm{d}s)$, respectively, so that—after division by $\hbar$—equation (20) can be rewritten more compactly as

$$\int_\gamma \omega_0^\theta - \int_{\gamma'} \omega_0^\theta = \int_\gamma \omega_0 - \int_{\gamma'} \omega_0.$$

Here use is made of the fact that the integrals with integrands $\mathcal{L}_0'^\theta$ and $\mathcal{L}'_0$ are the respective evaluations of ω_0^θ and ω_0 along the curve γ'. Using the property that negative signs preceding line integrals over curves reverse the orientation of the curves (i.e., the direction of integration), the last equation becomes

$$\int_C \omega_0^\theta = \int_C \omega_0,$$

where C is the simple smooth closed curve that is the union of γ and $-\gamma'$. Thus, it can be concluded that *for any two last point equivalent paths in* $\mathcal{H}$, *the value of the associated PFS 1-form* ω_0 *on* C (i.e., $\int_C \omega_0$) *is invariant under canonical pointed weak energy gauge transformations*—or equivalently—*its value is invariant under the replacement* $\omega_0 \to \omega_0^\theta$ (this is an immediate consequence of equation (16) and the fact that $\int_C \mathrm{d}\theta_t = 0$).

The path independence property of equation (9) can be used to evaluate this invariant. In particular, since the curves γ and γ' have the same first and last points, then it must be necessarily true that *for any two last point equivalent paths in* $\mathcal{H}$

$$\int_\gamma \omega_0 = \int_{\gamma'} \omega_0.$$

Upon rearrangement this becomes

$$\int_\gamma \omega_0 - \int_{\gamma'} \omega_0 = 0,$$

so that

$$\int_C \omega_0 = 0. \tag{21}$$

An interesting relationship between these line integrals for proper evolutions in $\mathcal{H}$ and geometric phase can be established by examining the properties of these line integrals that correspond to lifts of a simple closed curve Ω in the projective space $\mathcal{P}$ of $\mathcal{H}$ over the time interval $[0, \tau]$ with $[\psi(0)] = [\psi(\tau)]$. Let the lift of Ω be such that its image in $\mathcal{B}$ is smooth and simple. When the lift of Ω is closed, then $|\psi(0)\rangle = |\psi(\tau)\rangle$ and its image in $\mathcal{B}$ is a loop C with $(0, 0)$ as its first and last point and which intersects the χ and s axes only at the origin. In this case, equation (21) obviously applies. However, if the lift of Ω is not closed, then $|\psi(\tau)\rangle = e^{i\lambda}|\psi(0)\rangle$ and the image of the lift in $\mathcal{B}$ is a path γ which has $(\chi(\tau), 0) = (\lambda, 0)$ as its last point. It then follows from equation (9) that

$$\int_\gamma \omega_0 = f(\lambda, 0) = \lambda.$$

Note that equation (21) still holds in this case because γ' is the linear path along the χ axis with first point $(0, 0)$ and last point $(\lambda, 0)$ such that C is the union of γ and $-\gamma'$ and $\int_{\gamma'} \omega_0 = \lambda$.

For the special case that the lift is a horizontal lift, then λ is the geometric phase and

$$\int_\gamma \omega_0 = \int_\Omega \mathcal{A}, \tag{22}$$

where $\mathcal{A}$ is the associated Aharonov–Anandan connection 1-form [10]. Thus, it can be concluded from this that *for each such horizontal lift of an Ω in $\mathcal{P}$ there exists a path γ in $\mathcal{B}$ for which the last equation is satisfied*.

7. Examples

Before concluding this paper, it is instructive to briefly consider several simple examples which illustrate aspects of the above theory. The first example examines the relationship between pointed weak energy and irreversible decay processes and describes the evolutionary path followed by such a decaying state in PFS configuration space. The second example employs Grover's quantum search algorithm to demonstrate the utility of PFS configuration space for describing the discrete evolutionary steps of a quantum state evolving under the repeated action of an operator.

7.1. Irreversible decay processes

Consider the state

$$|\psi(t)\rangle = c_j(t)\exp\left(-i\frac{E_j t}{\hbar}\right)|\phi_j\rangle + \int c(\xi, t)\exp\left(-i\frac{Et}{\hbar}\right)|\xi\rangle\, d\xi,$$

where

$$c_j(t) = \exp\left(-\left[\frac{\Gamma}{2} + i\frac{\delta E}{\hbar}\right]t\right), \qquad \Gamma \in \mathcal{R}, \quad \delta E \in \mathcal{R},$$
$$c(\xi, 0) = 0, \qquad \langle\phi_j|\phi_j\rangle = 1, \qquad \langle\phi_j|\xi\rangle = 0,$$

and

$$\langle\xi|\xi'\rangle = \delta(\xi - \xi'),$$

which describes the coupling of a system initially in state $|\phi_j\rangle$ to the continuum and its irreversible decay thereto (the reader is invited to consult Cohen-Tannoudji *et al* [11] for additional details concerning this state).

For this state $|\psi(0)\rangle = |\phi_j\rangle$ so that

$$\langle\psi(t)|\psi(0)\rangle = c_j^*(t)\exp\left(i\frac{E_j t}{\hbar}\right) = \exp\left(-\frac{\Gamma}{2}t + i\left(\frac{E_j + \delta E}{\hbar}\right)t\right).$$

Comparison of this result with that of equation (10) yields

$$\mathcal{L}_0 = E_j + \delta E + \mathrm{i}\hbar\frac{\Gamma}{2}.$$

Thus, *the pointed weak energy associated with this decay process is a constant of the motion* and the probability that the state is still in the initial state at time $t > 0$ is given by

$$\Pr(s) \equiv |\langle\psi(t)|\psi(0)\rangle|^2 = \exp\left(-\frac{2}{\hbar}\int_0^t \mathrm{Im}\,\mathcal{L}_0\,\mathrm{d}t'\right) = \mathrm{e}^{-\Gamma t}.$$

The initial state $|\psi(0)\rangle = |\phi_j\rangle$ has a finite lifetime of $\Gamma^{-1} = \frac{\hbar}{2}(\mathrm{Im}\,\mathcal{L}_0)^{-1}$ and the probability $\Pr(s)$ decreases exponentially and irreversibly from unity and approaches zero as $t \to \infty$.

In addition,

$$\chi(t) = \left(\frac{E_j + \delta E}{\hbar}\right)t, \qquad (23)$$

$$s(t) = 2(1 - \mathrm{e}^{-\Gamma t})^{\frac{1}{2}}, \qquad (24)$$

$$\dot{s}(t) = \Gamma\,\mathrm{e}^{-\Gamma t}(1 - \mathrm{e}^{-\Gamma t})^{-\frac{1}{2}},$$

$$p_\chi = \hbar,$$

and

$$p_s = \frac{\mathrm{i}\hbar}{2}\,\mathrm{e}^{\Gamma t}(1 - \mathrm{e}^{-\Gamma t})^{\frac{1}{2}}.$$

From this it is seen that the evolutionary path in $\mathcal{B}$ is described parametrically by equations (23) and (24) with $s \to 2$ as $t \to \infty$. Also, whereas the rate of change of χ and p_χ are constant with time, $\dot{s} \to 0$ and $p_s \to \mathrm{i}\infty$ as $t \to \infty$. These, of course, are the conditions for $\mathcal{L}_0$ to be a constant of the motion.

7.2. Grover's quantum search algorithm

Grover's n qubit search algorithm [12] involves the iterative application of a rotation operator $\widehat{G}$ to an initial state $|\psi_0\rangle$ given by

$$|\psi_0\rangle = \cos\left(\frac{\theta}{2}\right)|\eta\rangle + \sin\left(\frac{\theta}{2}\right)|\sigma\rangle, \qquad (25)$$

with $|\eta\rangle = \left(\frac{1}{\sqrt{N-M}}\right)\sum_x'' |x\rangle$, $|\sigma\rangle = \left(\frac{1}{\sqrt{M}}\right)\sum_x' |x\rangle$, and $\cos\left(\frac{\theta}{2}\right) = \sqrt{\frac{N-M}{N}}$. Here $N = 2^n$, $1 \leqslant M \leqslant N$ is the number of search solutions, $\{|x\rangle : x = 0, 1, 2, \ldots, N-1\}$ is the set of orthonormal computational basis states, $\sum_x''$ denotes the sum over all $|x\rangle$ which are not search solutions and $\sum_x'$ denotes the sum over all $|x\rangle$ which are search solutions (so that $\langle\eta|\sigma\rangle = 0$). The k-fold application of $\widehat{G}$ to $|\psi_0\rangle$ yields the rotated state

$$|\psi_k\rangle \equiv \widehat{G}^k|\psi_0\rangle = \cos\left(\frac{2k+1}{2}\theta\right)|\eta\rangle + \sin\left(\frac{2k+1}{2}\theta\right)|\sigma\rangle, \qquad k \geqslant 0.$$

This state approaches the search solution state $|\sigma\rangle$ with repeated application of $\widehat{G}$ so that after a sufficient number of iterations a measurement of the computational basis will yield with high probability a search solution.

Observe that as θ continuously varies, then—since for each θ, $\mathrm{Im}\langle\psi_0|\,\mathrm{d}\psi_0\rangle = 0$—equation (25) defines the parallel transport of $|\psi_0\rangle$ along an evolutionary path α from $|\eta\rangle$ to $|\sigma\rangle$ in the associated Hilbert space $\mathcal{H}$. Furthermore, the projection $\Pi(\alpha)$ into $\mathcal{P}$ defines the shortest geodesic joining $[\psi_0]$ and $[\sigma]$ in $\mathcal{P}$ as measured by the Fubini-Study metric [13].

Consequently, each $|\psi_k\rangle$ is a point in α and its equivalent stepwise evolution in $\mathcal{P}$ is along the geodesic segment $\Pi(\alpha)$ (this may, in part, explain the computational efficiency of Grover's algorithm).

Now consider the image points of $|\psi_k\rangle$ in $\mathcal{B}$ under the pointed map Ψ_0 and the restriction $0 \leqslant k\theta < \frac{\pi}{2}$ (which is imposed to ensure that $|\psi_k\rangle \in \mathcal{H}_{\sim\perp}$). Clearly, $\Psi_0(|\psi_0\rangle) = (0, 0)$ and since

$$\varphi_k \equiv \langle\psi_k|\psi_0\rangle = \cos k\theta,$$

then

$$\chi_k = \arg \frac{\langle\psi_k|\psi_0\rangle}{|\langle\psi_k|\psi_0\rangle|} = 0$$

and

$$s_k = 2\sin k\theta.$$

The result $\chi_k = 0$ is consistent with the fact that $|\psi_k\rangle$ is parallel transported from $|\psi_0\rangle$ and implies that the image point in $\mathcal{B}$ of each $|\psi_k\rangle$ lies on the s-axis according to

$$\Psi_0(|\psi_k\rangle) = (0, 2\sin k\theta).$$

Thus, $\Psi_0(|\psi_k\rangle) \to (0, 2)$ as $k\theta \to \frac{\pi}{2}$ and the image points $\Psi_0(|\psi_k\rangle)$ evolve along a shortest path (i.e., a line segment) in $\mathcal{B}$.

The processing speed v_k in going from the kth to the $(k+1)$th step during the execution of Grover's algorithm can be defined as the difference $v_k = s_{k+1} - s_k = 4\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{2k+1}{2}\theta\right)$. When interpreted within this context, it can be seen from this that since v_k becomes smaller as $\frac{2k+1}{2}\theta \to \frac{\pi}{2}$, then the algorithmic processing 'slows' as $|\psi_k\rangle$ nears the solution state $|\sigma\rangle$. Also, for sufficiently small $k\theta$ it is easily determined that the pointed correlation amplitude decreases infinitesimally according to $\mathrm{d}\varphi = \varphi_{k+1} - \varphi_k \approx -k\theta^2$. Similarly, since $\mathrm{d}s = s_{k+1} - s_k \approx 2\theta$, then $\frac{\mathrm{i}}{2}\omega_{0_k}\varphi_k = -\frac{1}{2}(\tan k\theta)\,\mathrm{d}s \approx -k\theta^2$. Comparison of these results shows that equation (17) is valid for the infinitesimal regime of Grover's search algorithm and suggests that since $\varphi_{k+1} \approx \varphi_k - k\theta^2$, the effect of the $\omega_{0_k}\varphi_k$ interaction in this regime is to decrease the value of the pointed correlation amplitude with each iteration.

8. Concluding remarks

The classical mechanical nature of the quantum mechanical quantity called weak energy has previously been suggested by the similarity of the weak energy stationary action principle to Hamilton's principle [1]. A primary objective of this paper has been to further confirm this correspondence by identifying and studying in the PFS representation certain classical mechanical properties that are associated with pointed weak energy and its relationship to the evolution of a quantum state relative to its fixed initial state. It has been shown that these properties include the facts that: (i) the pointed weak energy satisfies the Euler–Lagrange equations for generalized PFS coordinates; (ii) a pointed weak energy stationary action principle can be stated that is a special case of the weak energy stationary action principle; and (iii) certain local $U(1)$ gauge transformations of quantum states are equivalent to transformations of the pointed weak energy and are analogues of gauge and canonical transformations of classical Lagrangian systems. An additional interesting consequence of item (iii) is that such transformations of the pointed weak energy identifies it with a pointed weak energy gauge potential which governs infinitesimal changes in the pointed correlation amplitude through an amplitude-gauge potential interaction.

In addition, the canonical and general canonical pointed weak energy gauge transformations, as well as the general pointed weak energy gauge potential transformation, were identified and the associated transformational invariance properties of the pointed weak energy stationary action principle, the Euler–Lagrange equations, the equation of motion for the pointed correlation amplitude, and the equation for the infinitesimal change in pointed correlation amplitude were discussed. It was noted that the transformational equivalences for the latter two equations hold true *only* because of the gauge transformation properties of the pointed weak energy and pointed weak energy gauge potential.

A zero-valued gauge invariant integral for last point equivalent paths expressed in terms of line integrals of the pointed weak energy gauge potential was also identified. This invariant and associated paths are useful for providing simple geometric interpretations in the Cartesian plane of phases related to lifts of closed curves in the projective Hilbert space. An especially interesting situation occurs when such lifts are horizontal. In this case, the pointed weak energy gauge potential captures the essence of the Aharonov–Anandan connection 1-form $\mathcal{A}$ in Hilbert space in the sense that such a lift defines a path in PFS configuration space over which the value of the pointed weak energy gauge potential is identical to that of $\mathcal{A}$ when it is evaluated over the associated closed curve in the projective Hilbert space.

Two simple examples were used to illustrate aspects of the theory. The first example used a state describing an irreversible decay process to develop a parametric description of the evolutionary path of the associated decay process in PFS configuration space. It was also shown that for this case the pointed weak energy is a constant of the motion. The second example employed Grover's quantum search algorithm to demonstrate the utility of PFS configuration space for studying the discrete evolutionary steps of a quantum system evolving under the repeated action of an operator. The accompanying analysis of this algorithm suggests that a geometric parallel transport property associated with the evolutionary steps of the process may provide a possible explanation for the algorithm's efficient performance.

Before closing, it is noted that this paper has identified several open questions that merit further investigation. These questions include the following: (1) Is there a physically meaningful fibre bundle representation that can be associated with the pointed weak energy gauge potential? (2) Is it possible to '*a priori*' identify paths γ in PFS configuration space that satisfy equation (22) and specify the closed paths Ω and their horizontal lifts in Hilbert space? (3) Is PFS configuration space useful for the study of chaotic quantum processes? (4) Are there useful insights that can be gained by generally using PFS configuration space to study the processing of quantum algorithms (other than, say, Grover's search algorithm)? and (5) What is the relationship between PFS configuration space and quantum control theory?

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