Annals of Mathematical Sciences and Applications
Volume 4, Number 2, 313–366, 2019

Orbit space curvature as a source of mass in quantum gauge theory

Vincent Moncrief, Antonella Marini, and Rachel Maitra

It has long been realized that the natural 'orbit space' for non-Abelian Yang-Mills dynamics (i.e., the reduced configuration space of gauge equivalence classes of spatial connections) is a *positively curved* (infinite dimensional) Riemannian manifold. Expanding upon this result I.M. Singer was led to propose that strict positivity of the corresponding Ricci tensor (computable from the rigorously defined curvature tensor through a suitable zeta function regularization procedure) could play a fundamental role in establishing that the associated Schrödinger operator admits a *spectral gap*. His argument was based on representing the (suitably regularized) kinetic term in the Schrödinger operator as a Laplace-Beltrami operator on this positively curved orbit space. In this article we revisit Singer's proposal and show how, when the contribution of the Yang-Mills (magnetic) potential energy is taken into account, the role of the original orbit space Ricci tensor is instead played by a certain 'Bakry-Émery Ricci tensor' computable from the ground state wave functional of the quantum theory. We next review the authors' ongoing *Euclidean-signature-semi-classical* program for deriving asymptotic expansions for such wave functionals and discuss how, by keeping the dynamical nonlinearities and non-Abelian gauge invariances fully intact at each level of the analysis, our approach surpasses that of conventional perturbation theory for the generation of such approximate wave functionals.

Though our main focus is on Yang-Mills theory we derive the corresponding orbit space curvature for scalar electrodynamics and prove that, whereas the Maxwell factor remains flat, the interaction naturally induces positive curvature in the (charged) scalar factor of the resulting orbit space. This has led us to the conjecture that such orbit space curvature effects could furnish a source of mass for ordinary Klein-Gordon type fields provided the latter are (minimally) coupled to gauge fields, even in the Abelian case.

AMS 2000 subject classifications: 81S10, 81T13, 83C45.
Keywords and phrases: Orbit space curvature, spectral gap, gauge theories.

arXiv: 1809.06318

1. Introduction

A fundamental question in quantum gauge theory is whether the Schrödinger operator for certain non-Abelian Yang-Mills fields admits a spectral gap. Such a gap, if it exists, could represent the energy difference between the actual vacuum state and that of the lowest energy 'glueball' states and confirm the expectation that massless gluons cannot propagate freely as photons do but must instead exhibit a form of 'color confinement'. It seems to be well understood that this question lies beyond the scope of conventional perturbation theory and will require a more global analytical treatment for its ultimate resolution.

Many years ago I.M. Singer proposed an elegant, geometrical approach to this fundamental problem based on the fact that the classical, reduced configuration space for Yang-Mills dynamics — namely the 'orbit space' of spatial connections modulo gauge transformations — has a naturally induced, *curved* Riemannian metric with everywhere non-negative sectional curvature [1]. The classical Hamiltonian for the reduced dynamics — a real-valued functional defined on the cotangent bundle of this orbit space — consists of a 'kinetic' term induced from the spatial integral of the square of the vectorial electric component of the full, spacetime Yang-Mills curvature tensor and a 'potential' term induced from the spatial integral of the square of its complementary, vectorial magnetic component. The non-vanishing curvature of the Riemannian metric defined by the kinetic term arises from the implementation of the Gauss-law constraint during the process of reduction to the quotient, orbit space and was independently computed by several investigators [1, 2, 3]. The classical reduced dynamics is thus that for a system point (namely a gauge equivalence class of spatial connections) moving on a positively curved, infinite dimensional manifold under the influence of a (non-negative) potential energy.

Upon canonical quantization the Schrödinger operator for this (pure Yang-Mills) dynamical system will thus include a kinetic term that, formally at least, encompasses the (negative[1]) Laplace-Beltrami operator for an infinite dimensional, curved Riemannian manifold — namely the orbit space alluded to above. Whereas the (covariant) Hessian of sufficiently smooth (wave) functionals can be rigorously defined in such infinite dimensional contexts, its associated trace need not make sense without some suitable regularization since the Hessian will not, in general, be trace class. Singer,

[1] We here adopt the usual physicists' sign convention for the definition of a Laplacian.

in particular, proposed an elegant zeta function regularization scheme to define the needed Laplacian [1].

A classical result in Riemannian geometry due to A. Lichnerowicz [4] shows that the Laplace operator for a complete, connected (finite-dimensional) Riemannian manifold necessarily exhibits a spectral gap provided that the Ricci tensor of this manifold is bounded, positively, away from zero.[2] Such a result however cannot be expected to extend, in any straightforward way at least, to the infinite dimensional manifolds arising in quantum Yang-Mills theory. First of all, as Singer pointed out, their Ricci tensors, which would result from taking traces of corresponding (rigorously computable) curvature tensors, are not in general well-defined — the curvature tensors in question not being trace class — and would require a suitable regularization for their meaningful formulation. Again Singer proposed zeta function regularization as an elegant means of accomplishing this. Some such regularization, however, is actually a desirable feature of the quantum procedure, at least in 4 spacetime dimensions, since it allows the introduction of a length scale into the quantum formalism. In the absence of such a scale no hypothetical spectral energy gap could even be expressed in terms of the naturally occurring parameters of the theory (Planck's constant, the speed of light and the Yang-Mills coupling constant).

Another difficulty with attempting to extend the Lichnerowicz argument to the infinite dimensional setting of interest here is that, thanks to the Bonnet-Myers theorem, one knows that a complete, finite dimensional Riemannian manifold with positive Ricci curvature bounded away from zero is necessarily compact [5]. For a connected such manifold the lowest eigenvalue of its associated (negative) Laplacian always vanishes and corresponds to a globally constant eigenfunction. That such an eigenfunction is nevertheless always normalizable follows from the manifold's compactness. The spectral gap referred to in Lichnerowicz's theorem is thus simply the lowest non-vanishing eigenvalue of the manifold's (negative) Laplacian which, in view of compactness, necessarily has a discrete spectrum.

Generalizations of Lichnerowicz's theorem have been established under less stringent conditions on the Ricci tensors provided that the manifolds under study have finite diameters [6, 7]. L. Andersson has proven that Riemannian Hilbert manifolds have finite diameters whenever their full sectional curvatures are positively bounded away from zero [8] but this result does not apply to the orbit space sectional curvatures of interest here since these

[2]It follows from the Bonnet-Myers theorem that such a manifold is necessarily compact [5].

latter admit (infinite dimensional) families of 2-planes on which they actually vanish. In any case the diameters of these Yang-Mills orbit spaces are known to be infinite [9].

The true, normalizable ground state wave functional must necessarily reflect the presence of the potential energy term in the Schrödinger operator. In Section 2 we show how to modify the original Lichnerowicz argument (in a finite dimensional setting) to allow for the occurrence of such a potential energy term and show that a corresponding gap estimate follows therefrom provided that a suitably defined 'Bakry-Émery Ricci tensor' is bounded positively away from zero. This Bakry-Émery Ricci tensor differs from the actual Ricci tensor by a term in the (covariant) Hessian of the logarithm of the true ground state wave function. Its positivity could hold on a flat or even negatively curved space and thus its applicability is not limited to manifolds of finite diameter.

Furthermore the natural integration measure arising in this (generalized Lichnerowicz) analysis includes the squared modulus of the ground state wave function itself so that the total space, even it it has infinite diameter, now has finite measure simply by virtue of the normalizability of the vacuum state. This should prove to be especially significant for any potential extensions to infinite dimensional problems wherein formal Lebesgue measures no longer make sense but for which normalizable vacuum state wave functionals are nevertheless expected to exist.

In Section 3 we discuss an ongoing program, under development by the authors, to derive asymptotic expansions for the wave functionals of certain interacting quantum field theories including, in particular Yang-Mills fields [10, 11, 12]. Our 'Euclidean signature semi-classical' analysis extends the applicability of certain elegant, microlocal methods to the case of bosonic field theories of renormalizable type. It has the significant advantage over conventional, Rayleigh-Schrödinger perturbation theory of keeping the nonlinearities and (if present) *non-Abelian* gauge invariances of an interacting system fully intact at every level of the analysis. Our expectation is that it should yield an asymptotic expansion for the needed, fully gauge invariant, logarithm of the ground state wave functional that is far superior to any attainable by conventional perturbation methods. The latter, by requiring an expansion in the Yang-Mills coupling constant, disturb both the nonlinear structure and the closely associated (non-Abelian) gauge invariance of the Yang-Mills dynamical system at the outset and attempt to reinstate those vital features only gradually, order-by-order in the expansion.

Though our main focus is on the Yang-Mills system we show in Section 4 how (non-vanishing) orbit space curvature also arises naturally through the

(minimal) coupling of a Maxwell field to a charged scalar field. In this case curvature arises only for the scalar factor of the (product) orbit space and not for the Maxwell factor which remains flat. We are thus led to conjecture that orbit space curvature could even serve as an independent source of mass for matter fields themselves provided that they are (minimally) coupled to (Abelian or non-Abelian) gauge fields.

Let ${}^{(4)}V := (\mathbb{R}^4, \eta)$, where

$$\eta = \eta_{\mu\nu}\, dx^\mu \otimes dx^\nu = -c^2\, dt \otimes dt + \sum_{i=1}^{3} dx^i \otimes dx^i, \tag{1}$$

designate Minkowski space expressed in a standard (Lorentz frame) coordinate system $\{x^\mu\} = \{ct, x^i\}$ and consider the Yang-Mills action functional (for a compact gauge group G) defined over domains Ω of the form $\Omega = I \times \mathbb{R}^3$ where $I = [t_0, t_1]$. Variation of this action with respect to the time component of the spacetime Yang-Mills connection field yields the so-called Gauss-law constraint equation which, for each fixed $t \in I$, may be viewed as an elliptic equation on $\mathbb{R}^3$ for this time component — a Lie-algebra valued function. If, with suitable boundary conditions imposed, one solves this constraint and substitutes the solution back into the action, the resulting reduced kinetic term (a quadratic form in the 'velocity' of the spatial connection) is found to be degenerate along gauge orbit directions but smooth, gauge invariant and positive definite in the transversal directions [1, 2, 3]. It thus follows that this kinetic term defines a smooth, Riemannian metric on the natural 'orbit space' of spatial connections modulo gauge transformations. This orbit space is (at least almost everywhere) itself a smooth, infinite dimensional manifold and provides the geometrically natural (reduced) configuration space for (classical) Yang-Mills dynamics.

A corresponding smooth *potential energy* functional is induced on this orbit space by the integral over $\mathbb{R}^3$ (at fixed t) of the square of the curvature of the spatial connection field — the 'magnetic' component of the curvature of the full spacetime connection field. A Legendre transformation leads in turn to the Hamiltonian functional for the classical dynamics which takes the 'standard' form of a sum of (curved space) kinetic and potential energies.

The sectional curvature of this reduced configuration space was independently computed in [1, 2, 3] and shown to be everywhere non-negative but almost everywhere non-vanishing whenever the gauge group G is non-Abelian. Though Singer discussed the need for a suitable regularization scheme to make sense of the formally (positively) divergent Ricci tensor of the orbit space metric, the actual form of such a regulated Ricci tensor

seems still to be unknown. It would be most interesting if a suitably defined Ricci tensor could be shown to be bounded, positively away from zero on this orbit space, especially inasmuch as we think it quite unlikely that the Bakry-Émery 'enhancement' of this tensor would nullify its (hypothetical) positivity properties but perhaps, more likely, complement them.[3] Furthermore, as we shall amplify near the end of Section 2, it seems quite plausible that strict positivity of the Bakry-Émery Ricci tensor, though sufficient for the implication of a spectral gap, is not absolutely necessary for this conclusion to hold.

2. Spectral gap estimates

A lower bound for the spectral gap of the Laplacian of a complete Riemannian manifold having strictly positive Ricci curvature was derived in a classic work by Lichnerowicz [4]. In view of the Bonnet-Myers theorem however such a manifold must be compact and, in particular, have its diameter bounded from above in terms of the assumed, positive lower bound on the Ricci tensor [5]. For compact manifolds the spectrum must of course be discrete, and thus exhibit a gap, but, in the absence of positive Ricci curvature, further geometrical information about the manifold would be needed to bound the actual gap. A flat torus, for example can have an arbitrarily large diameter and a corresponding, arbitrarily small gap.

For Schrödinger operators on the other hand, wherein the Laplacian is supplemented with a potential energy term, one can modify Lichnerowicz's argument so that the role of the Ricci tensor in the spectral gap estimate is now played by the so-called *Bakry-Émery Ricci tensor* which includes, indirectly, information about the potential energy function. For pure geometry problems, which need have no Schrödinger interpretation, the relevant Bakry-Émery tensor often arises from the study of so-called *metric measure spaces* wherein the natural Riemannian volume element is multiplied by a smooth positive function [13, 14].

In the Schrödinger context in particular, however, manifold compactness may no longer be needed since, in the revised argument, only positivity of the Bakry-Émery Ricci tensor is required to bound the spectral gap from below and, depending upon the nature of the potential energy involved, this condition may well hold in the presence of vanishing or even negative ordinary Ricci curvature. In an infinite dimensional, field theoretic

[3] This would be true for example if the relevant logarithm were (almost everwhere) convex.

setting on the other hand further possibilities may also arise in that positive Ricci curvature, which typically requires a suitable regularization to even be defined, need no longer imply manifold compactness. Setting such complications momentarily aside though, we sketch below the derivation of the relevant 'Bochner identity' for a conventional, kinetic-plus-potential Schrödinger operator defined over a (smooth, connected, complete and orientable) Riemannian n-manifold $\{M, g\}$.

Let Δ_g designate the covariant Laplacian (i.e., Laplace-Beltrami operator) given, in local coordinates for $\{M, g\}$ by

$$\Delta_g := \frac{1}{\mu_g}\,\partial_i(\mu_g g^{ij}\partial_j) \tag{2}$$

where $\mu_g := \sqrt{\det g}$, the natural volume element for the given manifold. If $V : M \to \mathbb{R}$ is a smooth function we define a corresponding Schrödinger (Hamiltonian) operator $\hat{H}$, for a 'particle' with mass $m > 0$, by

$$\hat{H} := -\frac{\hbar^2}{2m}\,\Delta_g + V \tag{3}$$

(with $\hbar := h/2\pi$ the reduced Planck constant) and assume that $\{M, g\}$ and V have been chosen so that $\hat{H}$ is well-defined and self-adjoint on a suitable domain in $L^2(M, g)$.

We also assume that the time-independent Schrödinger equation,

$$\hat{H}\Psi = E\Psi, \tag{4}$$

admits a (square integrable) ground state wave function,

$$\overset{(0)}{\Psi} = \overset{(0)}{N} e^{-\mathcal{S}/\hbar}, \tag{5}$$

with corresponding eigenvalue $E = \overset{(0)}{E} \in \mathbb{R}$, where $\mathcal{S} : M \to \mathbb{R}$ is a smooth function and $\overset{(0)}{N} \in \mathbb{C}$ a normalization constant (unique up to phase) chosen so that

$$\int_M \mu_g \overset{(0)}{\Psi}{}^{\dagger}\overset{(0)}{\Psi} d^n x = |\overset{(0)}{N}|^2 \int_M \mu_g e^{-2\mathcal{S}/\hbar} d^n x = 1. \tag{6}$$

Normalized excited state wave functions, orthogonal to the ground state, are expressible in the form

$$\overset{(*)}{\Psi} = \overset{(*)}{\varphi} e^{-\mathcal{S}/\hbar}, \tag{7}$$

with $\overset{(*)}{\varphi}: M \to \mathbb{C}$, and satisfy

$$\begin{aligned} \langle \overset{(*)}{\Psi} | \overset{(*)}{\Psi} \rangle &:= \int_M \mu_g \overset{(*)}{\Psi}{}^{\dagger} \overset{(*)}{\Psi} d^n x \\ &= \int_M \mu_g \overset{(*)}{\varphi}{}^{\dagger} \overset{(*)}{\varphi} e^{-2\mathcal{S}/\hbar} d^n x = 1 \end{aligned} \tag{8}$$

and

$$\langle \overset{(*)}{\Psi} | \overset{(0)}{\Psi} \rangle := \int_M \mu_g \overset{(*)}{\varphi}{}^{\dagger} \cdot \overset{(0)}{N} e^{-2\mathcal{S}/\hbar} d^n x = 0 \tag{9}$$

where $\overset{(*)}{\Psi}{}^{\dagger} = \overset{(*)}{\varphi}{}^{\dagger} e^{-\mathcal{S}/\hbar}$ is the complex conjugate of $\overset{(*)}{\Psi}$.

Noting that

$$\begin{aligned} (\hat{H} - \overset{(0)}{E}) \overset{(*)}{\Psi} &= (\hat{H} - \overset{(0)}{E}) (\overset{(*)}{\varphi} e^{-\mathcal{S}/\hbar}) \\ &= \frac{-\hbar^2}{2m} \left[\Delta_g \overset{(*)}{\varphi} - \frac{2}{\hbar} \mathcal{S}^{|k} \overset{(*)}{\varphi}_{|k} \right] e^{-\mathcal{S}/\hbar} \end{aligned} \tag{10}$$

where $\mathcal{S}^{|k} \overset{(*)}{\varphi}_{|k} := g^{k\ell} (\nabla_k \mathcal{S}) (\nabla_\ell \overset{(*)}{\varphi})$, with $|k = \nabla_k$ designating covariant differentiation with respect to g, we see that if $\overset{(*)}{\Psi}$ is an actual eigenstate of $\hat{H}$, with eigenvalue $E = \overset{(*)}{E} \in \mathbb{R}$, then

$$(\hat{H} - \overset{(0)}{E}) \overset{(*)}{\Psi} = (\overset{(*)}{E} - \overset{(0)}{E}) \overset{(*)}{\Psi} \tag{11}$$

or, equivalently

$$\frac{-\hbar^2}{2m} \left[\Delta_g \overset{(*)}{\varphi} - \frac{2}{\hbar} \mathcal{S}^{|k} \overset{(*)}{\varphi}_{|k} \right] = (\overset{(*)}{E} - \overset{(0)}{E}) \overset{(*)}{\varphi}. \tag{12}$$

The operator

$$\hat{\mathcal{H}} := -\frac{\hbar^2}{2m} \left[\Delta_g - \frac{2}{\hbar} \mathcal{S}^{|k} \nabla_k \right], \tag{13}$$

which is self-adjoint with respect to the measure $\mu_g e^{-2\mathcal{S}/\hbar} d^n x$ on M, encompasses the so-called Bakry-Émery or Witten Laplacian (on functions) and its lowest nontrivial eigenvalue (in the case of a discrete spectrum) defines the spectral gap, $\overset{(1)}{E} - \overset{(0)}{E}$ of principal interest herein.

From equations (10–12) one finds that

$$
\begin{aligned}
(\overset{(*)}{E} - \overset{(0)}{E}) \int_M \overset{(*)}{\Psi}{}^{\dagger} \overset{(*)}{\Psi} \mu_g d^n x &= (\overset{(*)}{E} - \overset{(0)}{E}) \int_M \overset{(*)}{\varphi}{}^{\dagger} \overset{(*)}{\varphi} e^{-2\mathcal{S}/\hbar} \mu_g d^n x \\
&= \frac{\hbar^2}{2m} \int_M \mu_g e^{-2\mathcal{S}/\hbar} \overset{(*)}{\varphi}{}^{\dagger}_{|k} \overset{(*)}{\varphi}{}^{|k} d^n x \\
&\quad - \frac{\hbar^2}{2m} \int_M \mu_g \left(\overset{(*)}{\varphi}{}^{\dagger} \overset{(*)}{\varphi}{}^{|k} e^{-2\mathcal{S}/\hbar} \right)_{|k} d^n x \\
&= \frac{\hbar^2}{2m} \int_M \mu_g e^{-2\mathcal{S}/\hbar} \overset{(*)}{\varphi}{}^{\dagger}_{|k} \overset{(*)}{\varphi}{}^{|k} d^n x
\end{aligned} \tag{14}
$$

where the vanishing of the integral of the divergence follows from the (assumed) self-adjoincy of $\hat{H} - \overset{(0)}{E}$. In view of its assumed orthogonality to the ground state $\overset{(*)}{\varphi}$ cannot be constant and thus (14) immediately implies that $(\overset{(*)}{E} - \overset{(0)}{E}) > 0$ (in this case of a discrete spectrum). To put a quantitative lower bound on this gap however requires a further argument.

To this end define, for any smooth function $\tilde{\varphi} : M \to \mathbb{C}$, the quantity

$$
\tilde{\mathcal{Q}}_{\tilde{\varphi}} := g^{ij} (\nabla_i \tilde{\varphi}^{\dagger}) (\nabla_j \tilde{\varphi}) e^{-2\mathcal{S}/\hbar} \tag{15}
$$

and apply the covariant Laplacian thereto. The result can be expressed as

$$
\begin{aligned}
\Delta_g \tilde{Q}_{\tilde{\varphi}} &= \nabla^k \nabla_k (g^{ij} \tilde{\varphi}^{\dagger}_{|i} \tilde{\varphi}_{|j} e^{-2\mathcal{S}/\hbar}) \\
&= -2 \left(\frac{2m}{\hbar^2} \right)^2 \left[(\hat{H} - \overset{(0)}{E}) (\tilde{\varphi}^{\dagger} e^{-\mathcal{S}/\hbar}) \right] \left[(\hat{H} - \overset{(0)}{E}) (\tilde{\varphi} e^{-\mathcal{S}/\hbar}) \right] \\
&\quad + 2 \tilde{\varphi}^{\dagger}_{|ij} \tilde{\varphi}^{|ij} e^{-2\mathcal{S}/\hbar} + 2 \mathcal{R}_{ij} \tilde{\varphi}^{\dagger|i} \tilde{\varphi}^{|j} e^{-2\mathcal{S}/\hbar} + \frac{4}{\hbar} \mathcal{S}^{|ij} \tilde{\varphi}^{\dagger}_{|i} \tilde{\varphi}_{|j} e^{-2\mathcal{S}/\hbar} \\
&\quad + \left\{ \tilde{\varphi}^{|j} e^{-2\mathcal{S}/\hbar} \left(\tilde{\varphi}^{\dagger|k}_{|k} - \frac{2}{\hbar} \mathcal{S}^{|k} \tilde{\varphi}^{\dagger}_{|k} \right) + \tilde{\varphi}^{\dagger|j} e^{-2\mathcal{S}/\hbar} \left(\tilde{\varphi}^{|k}_{|k} - \frac{2}{\hbar} \mathcal{S}^{|k} \tilde{\varphi}_{|k} \right) \right. \\
&\quad \left. - \frac{2}{\hbar} \mathcal{S}^{|j} \tilde{\varphi}^{\dagger|k} \tilde{\varphi}_{|k} e^{-2\mathcal{S}/\hbar} \right\}_{|j}
\end{aligned} \tag{16}
$$

where the Ricci tensor, $\mathcal{R}_{ij} dx^i \otimes dx^j$, of the metric g has arisen from the commutation of covariant derivatives followed by contraction of the resultant curvature tensor. This formula is the 'Bochner identity' referred to above and it naturally incorporates the Bakry-Émery Ricci tensor $\mathcal{R}^{\mathcal{S}} = \mathcal{R}^{\mathcal{S}}_{ij} dx^i \otimes dx^j$

defined by

$$\mathcal{R}^{\mathcal{S}}_{ij} = \mathcal{R}_{ij} + \frac{2}{\hbar}\mathcal{S}_{|ij}. \tag{17}$$

Taking, for the moment, $\tilde{\varphi}$ to have compact support and integrating (16) over M one arrives at

$$\begin{aligned} &2\left(\frac{2m}{\hbar^2}\right)^2 \int_M \mu_g \left[(\hat{H} - \overset{(0)}{E})(\tilde{\varphi}^\dagger e^{-\mathcal{S}/\hbar})\right]\left[(\hat{H} - \overset{(0)}{E})(\tilde{\varphi} e^{-\mathcal{S}/\hbar})\right] d^n x \\ &= \int_M \mu_g \left\{2\left(\mathcal{R}_{ij} + \frac{2}{\hbar}\mathcal{S}_{|ij}\right)\tilde{\varphi}^{\dagger|i}\tilde{\varphi}^{|j} e^{-2\mathcal{S}/\hbar} + 2\tilde{\varphi}^\dagger_{|ij}\tilde{\varphi}^{|ij} e^{-2\mathcal{S}/\hbar}\right\} d^n x \\ &= 2\left(\frac{2m}{\hbar^2}\right)^2 \int_M \mu_g \left\{(\tilde{\varphi}^\dagger e^{-\mathcal{S}/\hbar})(\hat{H} - \overset{(0)}{E})^2(\tilde{\varphi} e^{-\mathcal{S}/\hbar})\right\} d^n x \end{aligned} \tag{18}$$

where the final equality results from the self-adjoincy of the operator $\hat{H} - \overset{(0)}{E}$.

If now $\overset{(1)}{\Psi} = \overset{(1)}{\varphi} e^{-\mathcal{S}/\hbar}$ is an eigenstate of $\hat{H}$ with eigenvalue $\overset{(1)}{E}$ corresponding (in this case of a discrete spectrum) to a minimally excited state then one can approximate this state by a sequence of functions of compact support, $\tilde{\Psi}_\ell = \tilde{\varphi}_\ell e^{-\mathcal{S}/\hbar} \xrightarrow[\ell\to\infty]{} \overset{(1)}{\Psi} = \overset{(1)}{\varphi} e^{-\mathcal{S}/\hbar}$, the space of which densely filling the relevant Hilbert space, and conclude from (18) that, in the limit, $\overset{(1)}{\Psi} = \overset{(1)}{\varphi} e^{-\mathcal{S}/\hbar}$ satisfies

$$\begin{aligned} &2\left(\frac{2m}{\hbar^2}\right)^2 (\overset{(1)}{E} - \overset{(0)}{E})^2 \int_M \mu_g \overset{(1)}{\Psi}{}^\dagger \overset{(1)}{\Psi} d^n x \\ &= 2\left(\frac{2m}{\hbar^2}\right)^2 (\overset{(1)}{E} - \overset{(0)}{E})^2 \int_M \mu_g \overset{(1)}{\varphi}{}^\dagger \overset{(1)}{\varphi} e^{-2\mathcal{S}/\hbar} d^n x \\ &= \int_M \mu_g \left\{2\left(\mathcal{R}^{ij} + \frac{2}{\hbar}\mathcal{S}^{|ij}\right)\overset{(1)}{\varphi}{}^\dagger_{|i}\overset{(1)}{\varphi}_{|j} e^{-2\mathcal{S}/\hbar} + 2\overset{(1)}{\varphi}{}^\dagger_{|ij}\overset{(1)}{\varphi}{}^{|ij} e^{-2\mathcal{S}/\hbar}\right\} d^n x \\ &= 2\left(\frac{2m}{\hbar^2}\right)(\overset{(1)}{E} - \overset{(0)}{E}) \int_M \mu_g \overset{(1)}{\varphi}{}^\dagger_{|k}\overset{(1)}{\varphi}{}^{|k} e^{-2\mathcal{S}/\hbar} d^n x \end{aligned} \tag{19}$$

where the last equality results from applying (14) to the case at hand.

Since $\overset{(1)}{\Psi} = \overset{(1)}{\varphi} e^{-\mathcal{S}/\hbar}$ is orthogonal to the ground state $\overset{(1)}{\varphi}$ cannot be constant

and thus one gets from (19) that

(20)

$$
\begin{aligned}
&(\overset{(1)}{E} - \overset{(0)}{E}) \\
&\quad = \left\{ \frac{\dfrac{\hbar^2}{2m}\displaystyle\int_M \mu_g \left\{ \left(\mathcal{R}^{ij} + \frac{2}{\hbar}\mathcal{S}^{|ij} \right) \overset{(1)}{\varphi}{}^{\dagger}_{|i} \overset{(1)}{\varphi}{}_{|j} e^{-2\mathcal{S}/\hbar} + \overset{(1)}{\varphi}{}^{\dagger}_{|ij} \overset{(1)}{\varphi}{}^{|ij} e^{-2\mathcal{S}/\hbar} \right\} d^n x}{\displaystyle\int_M \mu_g \left\{ \overset{(1)}{\varphi}{}^{\dagger}_{|k} \overset{(1)}{\varphi}{}^{|k} e^{-2\mathcal{S}/\hbar} \right\} d^n x} \right\} \\
&\quad \geq \frac{\dfrac{\hbar^2}{2m}\displaystyle\int_M \mu_g \left\{ e^{-2\mathcal{S}/\hbar} \left(\mathcal{R}^{ij} + \frac{2}{\hbar}\mathcal{S}^{|ij} \right) \overset{(1)}{\varphi}{}^{\dagger}_{|i} \overset{(1)}{\varphi}{}_{|j} \right\} d^n x}{\displaystyle\int_M \mu_g \left\{ e^{-2\mathcal{S}/\hbar} \overset{(1)}{\varphi}{}^{\dagger}_{|k} \overset{(1)}{\varphi}{}^{|k} \right\} d^n x} \\
&\quad \geq \inf_{\tilde{\varphi} \in \mathcal{A}} \frac{\dfrac{\hbar^2}{2m}\displaystyle\int_M \mu_g \left\{ e^{-2\mathcal{S}/\hbar} \mathcal{R}^{\mathcal{S}}_{ij} \tilde{\varphi}^{\dagger|i} \tilde{\varphi}^{|j} \right\} d^n x}{\displaystyle\int_M \mu_g \left\{ e^{-2\mathcal{S}/\hbar} \tilde{\varphi}^{\dagger}_{|k} \tilde{\varphi}^{|k} \right\} d^n x}
\end{aligned}
$$

where $\mathcal{A}$ is the space of smooth functions on M satisfying

$$\int_M \mu_g e^{-2\mathcal{S}/\hbar} \tilde{\varphi}^{\dagger} \tilde{\varphi} d^n x = 1 \tag{21}$$

and

$$\int_M \mu_g e^{-2\mathcal{S}/\hbar} \tilde{\varphi}^{\dagger} \cdot 1 d^n x = 0. \tag{22}$$

From the foregoing it follows that if the Bakry-Émery Ricci tensor, $\mathcal{R}^{\mathcal{S}} = \mathcal{R}^{\mathcal{S}}_{ij} dx^i \otimes dx^j$ satisfies the global positivity condition,

$$\mathcal{R}^{\mathcal{S}}_{ij} v^i v^j \geq \frac{1}{\ell_o^2} g_{ij} v^i v^j, \tag{23}$$

for an arbitrary vector field $\mathbf{v} = v^i \partial_i$ on M, for some constant $\ell_o > 0$ (with the dimensions of length), then the spectral gap satisfies

$$\overset{(1)}{E} - \overset{(0)}{E} \geq \frac{\hbar^2}{2m} \frac{1}{\ell_o^2}. \tag{24}$$

As a special case of the above consider a (multi-dimensional) *harmonic* oscillator on Euclidean $\mathbb{R}^n$ with oscillation frequencies $0 < \omega_1 \leq \omega_2 \leq \cdots \leq$

ω_n along the various Cartesian coordinate axes. The function $\mathcal{S}$ is then given by

$$\mathcal{S} = \frac{1}{2}\sum_{j=1}^{n} m\omega_j (x^j)^2 \tag{25}$$

so that

$$\frac{2}{\hbar}\frac{\partial^2 \mathcal{S}}{\partial x^j \partial x^\ell} = \frac{2m}{\hbar}\omega_j \delta_{j\ell} \qquad \text{(no sum on } j\text{)} \tag{26}$$

and thus that

$$\mathcal{R}^{\mathcal{S}}_{j\ell} v^j v^\ell \geq \frac{2m\omega_1}{\hbar}\delta_{j\ell} v^j v^\ell \tag{27}$$

It follows from (24), taking $\frac{1}{\ell_o^2} = \frac{2m\omega_1}{\hbar}$, that

$$\overset{(1)}{E} - \overset{(0)}{E} \geq \hbar\omega_1. \tag{28}$$

That the gap estimate is sharp in this case results from the fact that $\overset{(1)}{\varphi}$ is a first order Hermite polynomial in x^1 which, being linear in x^1, satisfies $\overset{(1)}{\varphi}_{|ij} = 0$.

In the foregoing we assumed that the excited state spectrum was discrete. Suppose instead that it is continuous with $\overset{(1)}{E} > \overset{(0)}{E}$ designating the infimum of the (continuous) excited state spectrum. From the spectral decomposition theorem [15] it follows that, for any $\epsilon > 0$, there will exist normalizable states, Ψ_ϵ, orthogonal to the ground state, satisfying

$$\int_M \mu_g \Psi_\epsilon^\dagger (\hat{H} - \overset{(1)}{E})\Psi_\epsilon d^n x \geq 0, \tag{29}$$

$$\int_M \mu_g \left\{ \left[(\hat{H} - \overset{(1)}{E})\Psi_\epsilon\right]^\dagger \left[(\hat{H} - \overset{(1)}{E})\Psi_\epsilon\right] \right\} d^n x \leq \epsilon^2 \int_M \mu_g \Psi_\epsilon^\dagger \Psi_\epsilon d^n x \tag{30}$$

and

$$\int_M \mu_g \Psi_\epsilon^\dagger \overset{(0)}{\Psi} d^n x = 0 \tag{31}$$

Note that the imposition of (31) is essential for the validity of (29) since otherwise one could simply take $\Psi_\epsilon \to \overset{(0)}{\Psi}$ to get a counterexample. One can

assume for convenience though that Ψ_ϵ has compact support and is smooth since the space of such functions is dense in the Hilbert space of interest.

From the Schwarz inequality one has, upon appealing to (30), that

(32)
$$\begin{aligned} 0 &\leq \int_M \mu_g \Psi_\epsilon^\dagger (\hat{H} - \overset{(1)}{E}) \Psi_\epsilon d^n x \\ &\leq \Big(\int_M \mu_g \Psi_\epsilon^\dagger \Psi_\epsilon d^n x\Big)^{1/2} \left(\int_M \mu_g \left\{ \left[(\hat{H} - \overset{(1)}{E}) \Psi_\epsilon \right]^\dagger \left[(\hat{H} - \overset{(1)}{E}) \Psi_\epsilon \right] \right\} d^n x \right)^{1/2} \\ &\leq \epsilon \int_M \mu_g (\Psi_\epsilon^\dagger \Psi_\epsilon) d^n x \end{aligned}$$

Using the fact that $(\hat{H} - \overset{(1)}{E})$ is a real, self-adjoint operator it is easily verified that

(33)
$$\begin{aligned} &\int_M \mu_g \left\{ \left[(\hat{H} - \overset{(0)}{E}) \Psi_\epsilon \right]^\dagger \left[(\hat{H} - \overset{(0)}{E}) \Psi_\epsilon \right] \right\} d^n x \\ &\quad = \int_M \mu_g \left\{ \left[(\hat{H} - \overset{(1)}{E}) \Psi_\epsilon \right]^\dagger \left[(\hat{H} - \overset{(1)}{E}) \Psi_\epsilon \right] \right. \\ &\qquad \left. + (\overset{(1)}{E} - \overset{(0)}{E})^2 \Psi_\epsilon^\dagger \Psi_\epsilon + 2(\overset{(1)}{E} - \overset{(0)}{E}) \Psi_\epsilon^\dagger (\hat{H} - \overset{(1)}{E}) \Psi_\epsilon \right\} d^n x \\ &\quad \leq \epsilon^2 \int_M \mu_g \Psi_\epsilon^\dagger \Psi_\epsilon d^n x + 2(\overset{(1)}{E} - \overset{(0)}{E}) \epsilon \int_M \mu_g \Psi_\epsilon^\dagger \Psi_\epsilon d^n x \\ &\qquad + (\overset{(1)}{E} - \overset{(0)}{E})^2 \int_M \mu_g \Psi_\epsilon^\dagger \Psi_\epsilon d^n x \\ &\quad = (\overset{(1)}{E} - \overset{(0)}{E} + \epsilon)^2 \int_M \mu_g \Psi_\epsilon^\dagger \Psi_\epsilon d^n x \end{aligned}$$

where, in the final step, we have applied (30) and (32).

Setting $\Psi_\epsilon = \varphi_\epsilon e^{-\mathcal{S}/\hbar}$ and combining (33) with (18), with $\tilde{\varphi} \to \varphi_\epsilon$, we get

(34)
$$\begin{aligned} &2 \left(\frac{2m}{\hbar^2} \right)^2 (\overset{(1)}{E} - \overset{(0)}{E} + \epsilon)^2 \int_M \mu_g (\Psi_\epsilon^\dagger \Psi_\epsilon) d^n x \\ &\quad \geq 2 \left(\frac{2m}{\hbar^2} \right)^2 \int_M \mu_g \left[(\hat{H} - \overset{(0)}{E}) \Psi_\epsilon^\dagger \right] \left[(\hat{H} - \overset{(0)}{E}) \Psi_\epsilon \right] d^n x \\ &\quad = 2 \left(\frac{2m}{\hbar^2} \right)^2 \int_M \mu_g \left\{ \left[(\hat{H} - \overset{(0)}{E}) (\varphi_\epsilon^\dagger e^{-\mathcal{S}/\hbar}) \right] \left[(\hat{H} - \overset{(0)}{E}) (\varphi_\epsilon e^{-\mathcal{S}/\hbar}) \right] \right\} d^n x \end{aligned}$$

$$= 2\int_M \mu_g \left\{ \left(\mathcal{R}_{ij} + \frac{2}{\hbar}\mathcal{S}_{|ij} \right) \varphi_\epsilon^{\dagger|i}\varphi_\epsilon^{|j} e^{-2\mathcal{S}/\hbar} + \varphi^\dagger_{\epsilon|ij}\varphi_\epsilon^{|ij} e^{-2\mathcal{S}/\hbar} \right\} d^n x$$
$$\geq 2\int_M \mu_g \left\{ \left(\mathcal{R}_{ij} + \frac{2}{\hbar}\mathcal{S}_{|ij} \right) \varphi_\epsilon^{\dagger|i}\varphi_\epsilon^{|j} e^{-2\mathcal{S}/\hbar} \right\} d^n x$$

Thus, assuming the Bakry-Émery bound (23), one arrives at

(35)
$$(\overset{(1)}{E} - \overset{(0)}{E} + \epsilon)^2 \int_M \mu_g (\Psi_\epsilon^\dagger \Psi_\epsilon) d^n x \geq \left(\frac{\hbar^2}{2m} \right)^2 \frac{1}{\ell_o^2} \int_M \mu_g \varphi_\epsilon^{\dagger|i}\varphi_\epsilon^{|j} g_{ij} e^{-2\mathcal{S}/\hbar} d^n x$$
$$= \frac{\hbar^2}{2m\ell_o^2} \int_M \mu_g \Psi_\epsilon^\dagger (\hat{H} - \overset{(0)}{E}) \Psi_\epsilon d^n x \geq \frac{\hbar^2}{2m\ell_0^2} (\overset{(1)}{E} - \overset{(0)}{E}) \int_M \mu_g \Psi_\epsilon^\dagger \Psi_\epsilon d^n x$$

where, in the final steps, we have appealed to (10) and (29) together with an integration by parts. Setting $\overset{(1)}{E} - \overset{(0)}{E} := \Delta E > 0$ we thus get from (35) that

$$\Delta E + 2\epsilon + \frac{\epsilon^2}{\Delta E} \geq \frac{\hbar^2}{2m\ell_o^2}, \qquad \forall\, \epsilon > 0 \tag{36}$$

and thus that

$$\Delta E \geq \frac{\hbar^2}{2m\ell_0^2} \tag{37}$$

One might still wonder whether $\overset{(1)}{E} - \overset{(0)}{E} = 0$, i.e., with the normalizable ground state embedded at the bottom of a continuous excited state spectrum, is a remaining possibility. To exclude this, at least heuristically, (under the Bakry-Émery assumption (23)), note that (34) then gives

(38)
$$\int_M \mu_g \left\{ \varphi^\dagger_{\epsilon|ij}\varphi_\epsilon^{|ij} + \frac{1}{\ell_0^2}\varphi^\dagger_{\epsilon|j}\varphi_\epsilon^{|j} \right\} e^{-2\mathcal{S}/\hbar} d^n x \leq \left(\frac{2m}{\hbar^2} \right)^2 \epsilon^2 \int_M \mu_g \varphi_\epsilon^\dagger \varphi_\epsilon e^{-2\mathcal{S}/\hbar} d^n x$$

But a sequence, $\varphi_{1/\ell}$, of normalizable functions whose gradients converge to zero in $H^1(M, \mu_g e^{-2\mathcal{S}/\hbar})$-norm would have their gradients converging to zero almost everywhere and thus could not converge to a smooth limit orthogonal to the ground state.

Although global positivity of the Bakry-Émery Ricci tensor yields the quantitative lower bound (37) for the spectral gap it is almost surely not strictly needed for the existence of at least *some* gap. Suppose for example

that $\mathcal{R}^{\mathcal{S}} = \mathcal{R}^{\mathcal{S}}_{ij}\, dx^i \otimes dx^j$ actually vanishes on some lower dimensional variety embedded in M but is strictly positive on the complement. In view of the Hessian terms occurring in (20) and (34) one cannot simply arrive at a vanishing gap by assuming that the gradients of $\overset{(1)}{\varphi}$ and φ_ϵ respectively have their supports concentrated on the zero set of $\mathcal{R}^{\mathcal{S}}$. To convert this intuition to a quantitative estimate however would require a more detailed analysis which we shall not pursue here. It is worth emphasizing though that (23) is almost certainly only a sufficient condition for the existence of a spectral gap.

The foregoing has primarily been a rather straightforward application of some familiar techniques of geometric analysis (e.g. Bochner identities, the Schwarz inequality, Rayleigh quotient variational arguments, spectral theory) to the specific context of Schrödinger eigenvalue problems formulated on *curved manifolds*. In the mathematical literature on metric measure spaces and Bakry-Émery curvature (cf., [13, 14] and references cited therein) one often simply *specifies* the metric measure factor (the analogue of our $e^{-2\mathcal{S}/\hbar}$) and requires it to have certain desirable analytical properties (e.g., boundedness of $\mathcal{S}$ or of its gradient) depending upon the theorem to be proven (e.g., a generalization of the Bonnet-Myers theorem implying manifold compactness). For us on the other hand $\overset{(0)}{\Psi} := \overset{(0)}{N} e^{-\mathcal{S}/\hbar}$ is the ground state wave function for the Schrödinger eigenvalue problem under study and the 'background' Riemannian manifold $\{M, g\}$ is non-compact for the cases of most interest. Thus, for us, $\mathcal{S}$ is never freely specifiable but must satisfy the relevant differential equation and associated boundary conditions. In particular $\mathcal{S}$ will not be bounded (since this is incompatible with a normalizable ground state on a non-compact manifold of infinite volume) nor will it (as already seen in elementary examples) have bounded gradient. Thus, unfortunately, many of the hypotheses imposed upon $\mathcal{S}$ in the differential geometry literature are inappropriate for us and, of course, vice-versa.

Our ultimate aim, on the other hand, is to extend the ideas sketched above to the infinite dimensional 'configuration' spaces (typically Riemannian Hilbert manifolds) arising in the functional analytic approach to certain quantum field theories. The first step in this direction is, of course, to make sense of the Schrödinger operator itself. Whereas the covariant Hessian of a sufficiently smooth functional over such a space is still well-defined its corresponding metrical 'trace', or 'Laplacian', will not in general make sense without some suitable regularization since the Hessian under study will not, in general, be 'trace class'. There have however been a number of proposals in the literature for how best to regularize the formal functional Laplacians

that occur in the Schrödinger operators for bosonic quantum field theories, in particular gauge theories. Singer, for example, proposed an elegant 'zeta function' regularization scheme [1]. Later Hatfield [16] and quite recently Krug [17] have advanced alternative proposals, equally applicable to quantum gauge theories — the latter, in particular, involving a gauge invariant 'point splitting' technique.

If one tracks through the derivation above of the Bochner identity for the model, finite dimensional problem (16) and imagines extending this calculation to the field theoretic setting of primary interest herein, it becomes clear that the 'same' regularized trace operation that arises in defining the functional Laplacian will act on the curvature tensor of the configuration space metric g to yield its corresponding Ricci tensor. But the latter would also (as originally emphasized by Singer) not otherwise be well-defined since the curvature tensors of the relevant gauge theories are themselves *not trace class*. On the other hand the needed regularization procedure also plays the vital role (uniquely in 3+1 spacetime dimensions) of allowing a *length scale* to be introduced into the quantum formalism — a scale without which no hypothetical 'mass gap' could even be expressed in terms of the naturally occurring constants of the theory (Planck's constant, the speed of light and the Yang-Mills coupling constant).

Another key element in the finite dimensional model problem sketched above is the occurrence of numerous integrals over the Riemannian configuration manifold $\{M, g\}$. But thanks to the ubiquitous metric measure factor $e^{-2\mathcal{S}/\hbar}$ these integrals are *not* being taken with respect to the (Riemannian) Lebesgue measure $\mu_g d^n x$ but instead with respect to the measure $e^{-2\mathcal{S}/\hbar}\mu_g d^n x$ which for a normalizable ground state, will give a finite total measure for the non-compact manifold $\{M, g\}$. This distinction will prove to be crucial for our intended upgrade of the foregoing arguments to an infinite dimensional setting wherein Lebesgue measures no longer make sense but for which a normalizable ground state wave functional, together with its associated metric measure factor, is expected *to exist*. Furthermore the integrals to be carried out have much in common with the (Euclidean-signature) functional integrals arising in the Feynman path integral formalism with the important distinction that they only now involve the integrals over fields defined in *one lower dimension* than for the Feynman formalism. More precisely the integrals envisioned here would only be over 'instantaneous' field configurations defined over say $\mathbb{R}^3$ rather than over the (more technically problematic) spaces of field 'paths' defined over $\mathbb{R}^4$. This distinction is already dramatic in ordinary quantum mechanics wherein ordinary (finite

dimensional) Lebesgue integrals must be upgraded to genuine functional integrals in passing to the Feynman path integral formalism.

The naturally occurring metric measure factor $e^{-2\mathcal{S}/\hbar}$, which yields non-compact metric measure spaces $\{M, g, e^{-2\mathcal{S}/\hbar}\}$ of finite total measure, is the principal feature in our setup that allows us to contemplate extending the foregoing arguments to interesting infinite dimensional settings. Its absence was a key shortcoming in the original Singer proposal for exploiting Lichnerowicz type arguments for the existence of a spectral gap.[4] To carry out the needed extension (to field theoretic problems) in a technically precise way, on the other hand, would take us much further afield, analytically, than we are currently prepared to wander. Our intuition though is that such developments should be mathematically possible if one could gain sufficient control over the fundamental, logarithm functional $\mathcal{S}$. This latter step is, in large part, the aim of our Euclidean-signature semi-classical program which, for the convenience of the reader, we briefly review in the section to follow.

3. Euclidean signature semi-classical methods

3.1. Quantum mechanical systems

Elegant 'microlocal analysis' methods have long since been developed for the study of Schrödinger operators of the form (3) in the special cases for which $M \approx \mathbb{R}^n$, the metric g is flat and for which the potential energy function $V : M \to \mathbb{R}$ is of a suitable 'non-linear oscillatory' type [10, 18, 19, 20]. These methods[5] begin with an ansatz for the ground state wave function of the form

$$\overset{(0)}{\Psi}_{\hbar}(\mathbf{x}) = N_{\hbar}\, e^{-\mathcal{S}_{\hbar}(\mathbf{x})/\hbar} \tag{39}$$

[4]Singer, of course, was well aware of this limitation and does not explicitly mention the mass gap problem as motivation or the Lichnerowicz spectral gap estimate as a potentially useful tool in his original paper. He did however mention these both informally during a lecture at the Yale Mathematics Department in 1981 at which the senior author (V.M.) was present. Without this fortuitous clarification we would not have appreciated the potential for generalizing Singer's argument to allow for a normalizable ground state on a non-compact manifold.

[5]For reasons to be clarified below we here follow a recent reformulation of the traditional microlocal approach developed by the authors in [10].

and proceed to derive asymptotic expansions for the logarithm, $\mathcal{S}_\hbar : \mathbb{R}^n \to \mathbb{R}$, expressed formally as a power series in Planck's constant,

$$\mathcal{S}_\hbar(\mathbf{x}) \simeq \mathcal{S}_{(0)}(\mathbf{x}) + \hbar\mathcal{S}_{(1)}(\mathbf{x}) + \frac{\hbar^2}{2!}\mathcal{S}_{(2)}(\mathbf{x}) + \cdots + \frac{\hbar^n}{n!}\mathcal{S}_{(n)}(\mathbf{x}) + \cdots , \tag{40}$$

together with the associated ground state energy eigenvalue $\overset{(0)}{E}_\hbar$ expressed as

$$\overset{(0)}{E}_\hbar \simeq \hbar(\overset{(0)}{\mathcal{E}}_{(0)} + \hbar\overset{(0)}{\mathcal{E}}_{(1)} + \frac{\hbar^2}{2!}\overset{(0)}{\mathcal{E}}_{(2)} + \cdots + \frac{\hbar^n}{n!}\overset{(0)}{\mathcal{E}}_{(n)} + \cdots). \tag{41}$$

$N_\hbar$ is a corresponding (for us inessential) normalization constant which one could always evaluate at any (finite) level of the calculation.

When the above ansätze are substituted into the time-independent Schrödinger equation and the latter is required to hold order-by-order in powers of $\hbar$ the leading order term in the expansion (40) is found to satisfy an *inverted-potential-vanishing-energy* 'Hamilton-Jacobi' equation given by

$$\frac{1}{2m}g^{ij}\mathcal{S}_{(0),i}\mathcal{S}_{(0),i} - V = 0. \tag{42}$$

For a large class of (non-linear oscillatory) potential energy functions and when g is flat (with $g = \sum_{i=1}^n dx^i \otimes dx^i$) this equation can be proven to have a globally-defined, smooth, positive 'fundamental solution' that is unique up to a (trivial) additive constant. In particular this is true whenever

1. V is smooth, non-negative and has a unique global minimum attained at the origin of $\mathbb{R}^n$ where V vanishes,
2. V can be expressed as

$$V(x^1, \ldots, x^n) = \frac{1}{2}\sum_{i=1}^n m\,\omega_i^2 (x^i)^2 + A(x^1, \ldots, x^n) \tag{43}$$

where each of the 'frequencies' $\omega_i > 0$ for $i \in \{1, \ldots, n\}$ and wherein the smooth function $A : \mathbb{R}^n \to \mathbb{R}$ satisfies

$$A(0, \ldots, 0) = \frac{\partial A(0, \ldots, 0)}{\partial x^i} = \frac{\partial^2 A(0, \ldots, 0)}{\partial x^i \partial x^j} = 0 \quad \forall\, i, j\ \in \{1, \ldots, n\} \tag{44}$$

and the *coercivity* condition

$$A(x^1,\ldots,x^n) \geq -\frac{1}{2}m\sum_{i=1}^{n}\lambda_i^2(x^i)^2 \quad \forall\,(x^1,\ldots,x^n)\ \in \mathbb{R}^n \tag{45}$$

and for some constants $\{\lambda_i\}$ such that $\lambda_i^2 < \omega_i^2 \quad \forall\, i\ \in \{1,\ldots,n\}$, and

3. V satisfies the *convexity* condition

$$\sum_{i,j=1}^{n}\frac{\partial^2 V(x^1,\ldots,x^n)}{\partial x^i \partial x^j}\xi^i\xi^j \geq 0 \quad \forall\,(x^1,\ldots,x^n)\ \in \mathbb{R}^n \text{ and all } (\xi^1,\ldots,\xi^n)\ \in \mathbb{R}^n. \tag{46}$$

Since only the sufficiency of these conditions was actually established in [10] it is quite conceivable that a satisfactory *fundamental solution* to Eq. (42) exists under weaker hypotheses on the potential energy.

Our approach to proving the existence of a global, smooth fundamental solution to the (inverted-potential-vanishing-energy) Hamilton-Jacobi equation

$$\frac{1}{2m}\nabla\mathcal{S}_{(0)}\cdot\nabla\mathcal{S}_{(0)} - V = 0 \tag{47}$$

is quite different from that developed previously in the microlocal literature but has the advantage of being applicable to certain field theoretic problems whereas it seems the latter does not.[6]

To establish the existence of $\mathcal{S}_{(0)}$ we began by proving that the (inverted potential) action functional

$$\mathcal{I}_{ip}[\gamma] := \int_{-\infty}^{0}\left\{\frac{1}{2}m\sum_{i=1}^{n}\left[(\dot{x}^i(t))^2 + \omega_i^2(x^i(t))^2\right] + A\left(x^i(t),\ldots,x^n(t)\right)\right\}dt, \tag{48}$$

defined on an appropriate Sobolev space of curves $\gamma : (-\infty, 0] \to \mathbb{R}^n$, has a unique minimizer, $\gamma_{\mathbf{x}}$, for any choice of boundary data

$$\mathbf{x} = (x^1,\ldots,x^n) = \lim_{t\nearrow 0}\gamma_{\mathbf{x}}(t)\ \in\ \mathbb{R}^n \tag{49}$$

[6]The reasons for this apparent limitation are clarified in the discussion to follow.

and that this minimizer always obeys

$$\lim_{t\searrow -\infty} \gamma_{\mathbf{x}}(t) = (0, \ldots, 0). \tag{50}$$

We then showed that every such minimizing curve is smooth and satisfies the (*inverted potential*) Euler-Lagrange equation

$$m\frac{d^2}{dt^2}\gamma^i_{\mathbf{x}}(t) = \frac{\partial V}{\partial x^i}(\gamma_{\mathbf{x}}(t)) \tag{51}$$

with vanishing (inverted potential) energy

$$\begin{aligned} E_{ip}(\gamma_{\mathbf{x}}(t), \dot{\gamma}_{\mathbf{x}}(t)) &:= \frac{1}{2}m\sum_{i=1}^{n}(\dot{\gamma}^i_{\mathbf{x}}(t))^2 - V(\gamma_{\mathbf{x}}(t)) \\ &= 0 \quad \forall\, t\ \in (-\infty, 0] := I. \end{aligned} \tag{52}$$

Setting $\mathcal{S}_{(0)}(\mathbf{x}) := \mathcal{I}_{ip}[\gamma_{\mathbf{x}}]$ for each $\mathbf{x}\ \in \mathbb{R}^n$ we proceeded to prove, using the (Banach space) implicit function theorem, that the $\mathcal{S}_{(0)} : \mathbb{R}^n \to \mathbb{R}$, so-defined, satisfies the Hamilton-Jacobi equation

$$\frac{1}{2m}|\nabla \mathcal{S}_{(0)}|^2 - V = 0 \tag{53}$$

globally on $\mathbb{R}^n$ and regenerates the minimizers $\gamma_{\mathbf{x}}$ as the integral curves of its gradient (semi-)flow in the sense that

$$\begin{aligned} \frac{d}{dt}\gamma_{\mathbf{x}}(t) &= \frac{1}{m}\nabla \mathcal{S}_{(0)}(\gamma_{\mathbf{x}}(t)) \\ &\forall\, t\ \in I := (-\infty, 0] \ \text{ and} \\ &\forall\, \mathbf{x}\ \in \mathbb{R}^n \end{aligned} \tag{54}$$

Actually each such integral curves $\gamma_{\mathbf{x}} : I \to \mathbb{R}^n$ extends to a larger interval, $(-\infty, t^*(\gamma_{\mathbf{x}}))$ with $0 < t^*(\gamma_{\mathbf{x}}) \leq \infty\ \forall\ \mathbf{x}\ \in \mathbb{R}^n$ but since, in general, $t^*(\gamma_{\mathbf{x}}) < \infty$ we only have a semi-flow rather than a complete flow generated by $\frac{1}{m}\nabla \mathcal{S}_{(0)}$. Purely *harmonic* oscillations on the other hand (for which $A(x^1, \ldots, x^n) = 0$) are an exception, having $t^*(\gamma_{\mathbf{x}}) = \infty\ \forall\, \mathbf{x}\ \in \mathbf{R}^n$.

Among the additional properties established for $\mathcal{S}_{(0)}$ were the Taylor expansion formulas

$$\mathcal{S}_{(0)}(\mathbf{x}) = \frac{1}{2}m\sum_{i=1}^{n}\omega_i(x^i)^2 + O(|\mathbf{x}|^3), \tag{55}$$

$$\partial_j \mathcal{S}_{(0)}(\mathbf{x}) = m\omega_j x^j + O(|\mathbf{x}|^2) \tag{56}$$

and

$$\partial_j \partial_k \mathcal{S}_{(0)}(\mathbf{x}) = m\omega_k \delta^k_j + O(|\mathbf{x}|), \tag{57}$$

where here (exceptionally) no sum on the repeated index is to be taken, and the global lower bound

$$\mathcal{S}_{(0)}(\mathbf{x}) \geq \mathcal{S}^*_{(0)} := \frac{1}{2} m \sum_{i=1}^{n} \nu_i (x^i)^2 \tag{58}$$

where $\nu_i := \sqrt{\omega_i^2 - \lambda_i^2} > 0 \; \forall \; i \; \in \{1, \ldots, n\}$. Note especially that this last inequality guarantees that, in particular, $e^{-\mathcal{S}_{(0)}/\hbar}$ will always be normalizable on $\{\mathbb{R}^n, g = \sum_{i=1}^n dx^i \otimes dx^i\}$.

The higher order 'quantum corrections' to $\mathcal{S}^{(0)}$ (i.e., the functions $\mathcal{S}_{(k)}$ for $k = 1, 2, \ldots$) can now be computed through the systematic integration of a sequence of (first order, linear) 'transport equations', derived from Schrödinger's equation, along the integral curves of the gradient (semi-)flow generated by $\mathcal{S}_{(0)}$. The natural demand for global smoothness of these quantum 'loop corrections' forces the (heretofore undetermined) energy coefficients $\{\overset{(0)}{\mathcal{E}}_{(0)}, \overset{(0)}{\mathcal{E}}_{(1)}, \overset{(0)}{\mathcal{E}}_{(2)}, \ldots\}$ all to take on specific, computable values.

Excited states can now be analyzed by substituting the ansatz

$$\overset{(*)}{\Psi}_{\hbar}(\mathbf{x}) = \overset{(*)}{\phi}_{\hbar}(\mathbf{x}) e^{-\mathcal{S}_{\hbar}(\mathbf{x})/\hbar} \tag{59}$$

into the time independent Schrödinger equation and formally expanding the unknown wave functions $\overset{(*)}{\phi}_{\hbar}$ and energy eigenvalues $\overset{(*)}{E}_{\hbar}$ in powers of $\hbar$ via

$$\overset{(*)}{\phi}_{\hbar} \simeq \overset{(*)}{\phi}_{(0)} + \hbar \overset{(*)}{\phi}_{(1)} + \frac{\hbar^2}{2!} \overset{(*)}{\phi}_{(2)} + \cdots \tag{60}$$

$$\overset{(*)}{E}_{\hbar} \simeq \hbar \overset{(*)}{\mathcal{E}}_{\hbar} \simeq \hbar \left(\overset{(*)}{\mathcal{E}}_{(0)} + \hbar \overset{(*)}{\mathcal{E}}_{(1)} + \frac{\hbar^2}{2!} \overset{(*)}{\mathcal{E}}_{(2)} + \cdots \right) \tag{61}$$

while retaining the 'universal' factor $e^{-\mathcal{S}_{\hbar}(\mathbf{x})/\hbar}$ determined by the ground state calculations.

From the leading order analysis one finds that these excited state expansions naturally allow themselves to be labelled by an n-tuple $\mathbf{m} =$

$(m_1, m_2, \ldots, m_n)$ of non-negative integer 'quantum numbers', m_i, so that the foregoing notation can be refined to

$$\overset{(\mathbf{m})}{\Psi}{}_{\hbar}(\mathbf{x}) = \overset{(\mathbf{m})}{\phi}{}_{\hbar}(\mathbf{x}) e^{-\mathcal{S}_{\hbar}(\mathbf{x})/\hbar} \tag{62}$$

and

$$\overset{(\mathbf{m})}{E}{}_{\hbar} = \hbar \overset{(\mathbf{m})}{\mathcal{E}}{}_{\hbar} \tag{63}$$

with $\overset{(\mathbf{m})}{\varphi}{}_{\hbar}$ and $\overset{(\mathbf{m})}{\mathcal{E}}{}_{\hbar}$ expanded as before. Using methods that are already well-known from the microlocal literature [18] but slightly modified to accord with our setup [10] one can now compute all the coefficients $\{\overset{(\mathbf{m})}{\phi}{}_{(k)}, \overset{(\mathbf{m})}{\mathcal{E}}{}_{(k)}, k = 0, 1, 2 \ldots\}$ through the solution of a sequence of linear, first order transport equations integrated along the semi-flow generated by $\mathcal{S}_{(0)}$.

A key feature of this program, when applied to an n-dimensional *harmonic* oscillator, is that it regenerates all the well-known, *exact* results for both ground and excited states, correctly capturing not only the eigenvalues but the *exact eigenfunctions* as well [10, 18, 19]. One finds for example that the fundamental solution to the relevant (inverted-potential-vanishing-energy) Hamilton-Jacobi equation, for an n-dimensional oscillator (with mass m and (strictly positive) oscillation frequencies $\{\omega_i\}$) is given by

$$\mathcal{S}_{(0)}(\mathbf{x}) = \frac{1}{2} m \sum_{i=1}^{n} \omega_i (x^i)^2 \tag{64}$$

and that all higher order corrections to the logarithm of the ground state wave function vanish identically leaving the familiar gaussian

$$\overset{(0)}{\Psi}{}_{\hbar}(\mathbf{x}) = \overset{(0)}{N}{}_{\hbar}\, e^{-\frac{m}{2\hbar}\sum_{i=1}^{n} \omega_i (x^i)^2} \tag{65}$$

where $\mathbf{x} = (x^1, \ldots, x^n)$ and $\overset{(0)}{N}{}_{\hbar}$ is a normalization constant.

The construction of excited states begins with the observation that the only globally regular solutions to the corresponding, leading order 'transport equation' are composed of the monomials

$$\overset{(\mathbf{m})}{\phi}{}_{(0)}(\mathbf{x}) = (x^1)^{m_1} (x^2)^{m_2} \cdots (x^n)^{m_n}, \tag{66}$$

where $\mathbf{m} = (m_1, m_2, \ldots, m_n)$ is an n-tuple of non-negative integers with $|m| := \sum_{i=1}^{n} m_i > 0$, and proceeds after a finite number of unequivocal steps, to assemble the exact excited eigenstate prefactor

$$\begin{aligned} \overset{(\mathbf{m})}{\phi}{}_{\hbar}(\mathbf{x}) = \overset{(\mathbf{m})}{N}{}_{\hbar} H_{m_1}\left(\sqrt{\frac{m\omega_1}{\hbar}}x^1\right) H_{m_2}\left(\sqrt{\frac{m\omega_2}{\hbar}}x^2\right) \\ \cdots H_{m_n}\left(\sqrt{\frac{m\omega_n}{\hbar}}x^n\right) \end{aligned} \tag{67}$$

where H_k is the Hermite polynomial of order k (and $\overset{(\mathbf{m})}{N}{}_k$ is the corresponding normalization constant) [10, 18, 19].

While there is nothing especially astonishing about being able to rederive such well-known, exact results in a different way, we invite the reader to compare them with those obtainable via the textbook WKB methods of the physics literature [21, 22]. Even for purely *harmonic* oscillators conventional WKB methods yield only rather rough approximations to the wave functions and are, in any case, practically limited to one-dimensional problems and to those reducible to such through a separation of variables. The lesser known Einstein Brillouin Keller (or EBK) extension of the traditional semi-classical methods does apply to higher (finite-)dimensional systems but only to those that are completely integrable at the classical level [23]. In sharp contrast to these well-established approximation methods the (Euclidean signature[7]) semi-classical program that we are advocating here requires neither classical integrability nor (as we shall see) finite dimensionality for its implementation.

As was discussed in the concluding section of Ref. [10] our fundamental solution, $\mathcal{S}_{(0)}(\mathbf{x})$, to the (inverted-potential-vanishing-energy) Hamilton-Jacobi equation for a coupled system of nonlinear oscillators has a natural geometric interpretation. The graphs, in the associated phase space $T^*\mathbb{R}^n$, of its positive and negative gradients correspond precisely to the stable ($W^{\mathrm{s}}(p) \subset T^*\mathbb{R}^n$) and unstable ($W^{\mathrm{u}}(p) \subset T^*\mathbb{R}^n$) Lagrangian submanifolds of the assumed, isolated equilibrium point $p \in T^*\mathbb{R}^n$:

$$W^{\mathrm{u}}(p) = \left\{(\mathbf{x}, \mathbf{p}) : \mathbf{x} \in \mathbb{R}^n, \mathbf{p} = \nabla \mathcal{S}_{(0)}(\mathbf{x})\right\} \tag{68}$$

$$W^{\mathrm{s}}(p) = \left\{(\mathbf{x}, \mathbf{p}) : \mathbf{x} \in \mathbb{R}^n, \mathbf{p} = -\nabla \mathcal{S}_{(0)}(\mathbf{x})\right\} \tag{69}$$

[7]The significance of this qualifying expression will become clear when we turn to field theoretic problems.

Another result established for the aforementioned nonlinear oscillators of Ref. [10] is that the first quantum 'loop correction', $\mathcal{S}_{(1)}(x^1,\ldots,x^n)$, to the ('tree level') fundamental solution, $\mathcal{S}_{(0)}(x^1,\ldots,x^n)$, also has a natural geometric interpretation in terms of 'Sternberg coordinates' for the gradient (semi-)flow generated by this fundamental solution. Sternberg coordinates, by construction, linearize the Hamilton-Jacobi flow equation

$$m\frac{dx^i(t)}{dt} = \frac{\partial \mathcal{S}_{(0)}}{\partial x^i}(x^1(t),\ldots,x^n(t)) \tag{70}$$

to the form

$$\frac{dy^i(t)}{dt} = \omega_i y^i(t) \quad (\text{no sum on } i) \tag{71}$$

through, as was proven in Ref. [10], the application of a global diffeomorphism

$$\mu : \mathbb{R}^n \to \mu(\mathbb{R}^n) \subset \mathbb{R}^n = \left\{(y^1,\ldots,y^n)\right\}, \tag{72}$$

$$\mathbf{x} \mapsto \mu(\mathbf{x}) = \left\{y^1(\mathbf{x}),\ldots,y^n(\mathbf{x})\right\} \tag{73}$$

that maps $\mathbb{R}^n$ to a star-shaped domain $K = \mu(\mathbb{R}^n) \subset \mathbb{R}^n$ with $\mu^{-1}(K) \approx \mathbb{R}^n = \left\{(x^1,\ldots,x^n)\right\}$.

Though not strictly needed for the constructions of Ref. [10], Sternberg coordinates have the natural feature of generating a Jacobian determinant for the Hilbert-space integration measure that *exactly cancels* the contribution of the first quantum 'loop correction', $\mathcal{S}_{(1)}(\mathbf{x})$, to inner product calculations, taking, for example,

$$\begin{aligned}\left\langle \overset{(\mathbf{m})}{\Psi}, \overset{(\mathbf{m})}{\Psi} \right\rangle &:= \int_{\mathbb{R}^n} \left| \overset{(\mathbf{m})}{\Psi}(\mathbf{x}) \right|^2 d^n x \\ &= \int_{\mu(\mathbb{R}^n)} \left| \overset{(\mathbf{m})}{\Psi} \circ \mu^{-1}(\mathbf{y}) \right|^2 \sqrt{\det g_{**}(\mathbf{y})}\, d^n y\end{aligned} \tag{74}$$

to the form

$$\begin{aligned}\left\langle \overset{(\mathbf{m})}{\Psi}, \overset{(\mathbf{m})}{\Psi} \right\rangle = \int_{\mu(\mathbb{R}^n)} \left| \left[\overset{(\mathbf{m})}{\varphi}\, e^{\frac{-\mathcal{S}_{(0)}}{\hbar} - \frac{\hbar}{2!}\mathcal{S}_{(2)} + \cdots} \right] \circ \mu^{-1}(\mathbf{y}) \right|^2 \\ \sqrt{\det g_{**}(\mathbf{0})}\, d^n y\end{aligned} \tag{75}$$

where, in the last integral, the contribution of $\mathcal{S}_{(1)} \circ \mu^{-1}(\mathbf{y})$ to the wave function

$$\overset{(\mathbf{m})}{\Psi} \circ \mu^{-1}(\mathbf{y}) = \overset{(\mathbf{m})}{\varphi}\, e^{\frac{-\mathcal{S}_{(0)}}{\hbar} - \mathcal{S}_{(1)} - \frac{\hbar}{2!}\mathcal{S}_{(2)} \cdots} \circ \mu^{-1}(\mathbf{y}) \tag{76}$$

has precisely cancelled the non-Cartesian measure factor $\sqrt{\det g_{**}(\mathbf{y})}$, leaving the constant (Euclidean) factor $\sqrt{\det g_{**}(\mathbf{0})}$ in its place. Roughly speaking therefore, this role of $\mathcal{S}_{(1)}$ is to 'flatten out' the Sternberg coordinate volume element, reducing it to ordinary Lebesgue measure (albeit only over the star-shaped domain $\mu(\mathbb{R}^n)$), by exactly cancelling the Jacobian determinant that arises from the coordinate transformation.

For the nonlinear oscillators discussed in Ref. [10], Sternberg coordinates also have the remarkable property of allowing the leading order transport equation for *excited states* to be solved in closed form. Indeed, the regular solutions to this equation are comprised of the monomials

$$\overset{(\mathbf{m})}{\varphi}_{(0)}(\mathbf{y}) = (y^1)^{m_1}(y^2)^{m_2} \cdots (y^n)^{m_n} \tag{77}$$

wherein, precisely as for the harmonic case, the m_i are non-negative integers with $|\mathbf{m}| := \sum_{i=1}^{n} m_i > 0$. On the other hand the higher order corrections, $\left\{ \overset{(\mathbf{m})}{\varphi}_{(k)}(\mathbf{y}); k = 1, 2, \ldots \right\}$, to these excited state prefactors will not in general terminate at a finite order as they do for strictly *harmonic* oscillators but they are nevertheless systematically computable through the sequential integration of a set of well-understood linear transport equations [10, 18]. Formal expansions (in powers of $\hbar$) for the corresponding (ground and excited state) energy *eigenvalues* are uniquely determined by the demand for global regularity of the associated eigenfunction expansions. More precisely one finds, upon integrating the relevant transport equation at a given order, that the only potential breakdown of smoothness for the solution would necessarily occur at the 'origin' $\mathbf{x} = 0$ (chosen here to coincide with the global minimum of the potential energy) but that this loss of regularity can always be uniquely avoided by an appropriate choice of eigenvalue coefficient at the corresponding order.

A number of explicit calculations of the eigenfunctions and eigenvalues for a family of 1-dimensional *anharmonic* oscillators of quartic, sectic, octic, and dectic types were carried out in Ref. [10] and compared with the corresponding results from conventional Rayleigh/Schrödinger perturbation theory. To the orders considered (and, conjecturally, to all orders) our eigenvalue expansions agreed with those of Rayleigh/Schrödinger theory whereas

our wave functions, even at leading order, more accurately captured the more-rapid-than-gaussian decay known rigorously to hold for the exact solutions to these problems. For the quartic oscillator in particular our results strongly suggested that both the ground state energy eigenvalue expansion and its associated wave function expansion are Borel summable to yield natural candidates for the actual exact ground state solution and its energy.

Remarkably all of the integrals involved in computing the quantum corrections $\{\mathcal{S}_{(1)}, \mathcal{S}_{(2)}, \mathcal{S}_{(3)}, \cdots\}$ to $\mathcal{S}_{(0)}$ (up to the highest order computed in [10], namely $\mathcal{S}_{(25)}$) were expressible explicitly in terms of elementary functions for the *quartic* and *sectic* oscillators whereas for the octic and dectic cases some (but not all) of the quantum corrections required, in addition, hypergeometric functions for their evaluation. It seems plausible to conjecture that these patterns persist to all orders in $\hbar$ and thus, for the quartic and sectic[8] cases in particular, lead to formal expansions for $\mathcal{S}_{\hbar}$ in terms of elementary functions. The evidence supporting the conjectured Borel summability of this formal expansion in the quartic case is discussed in detail in Section V.A. of [10].

For the Lagrangians normally considered in classical mechanics it would not be feasible to define their corresponding action functionals over (semi-) infinite domains, as we have done, since the integrals involved, when evaluated on solutions to the Euler-Lagrange equations, would almost never converge. It is only because of the special nature of our problem, with its inverted potential energy function and associated boundary conditions, that we could define a convergent action integral for the class of curves of interest and use this functional to determine corresponding minimizers.

A remarkable feature of our construction, given the hypotheses of convexity and coercivity imposed upon the potential energy $V(\mathbf{x})$, is that it led to a *globally smooth* solution to the corresponding Hamilton-Jacobi equation. Normally the solutions to a Hamilton-Jacobi equation in mechanics fail to exist globally, even for rather elementary problems, because of the occurrence of caustics in the associated families of solution curves. For our problem however caustics were non-existent for the (semi-)flow generated by the gradient of $\mathcal{S}_{(0)}(\mathbf{x})$. The basic reason for this was the inverted potential character of the forces considered which led to the development of diverging (in the future time direction) solution curves having, in effect, uniformly positive Lyapunov exponents that served to prevent the occurrence of caustics altogether.

[8]These results were subsequently extended to significantly higher orders by P. Tang [24].

By contrast, the more conventional approach (in the physics literature) to semi-classical methods leads instead to a standard (non-inverted-potential-non-vanishing-energy) Hamilton-Jacobi equation for which, especially in higher dimensions, caustics are virtually unavoidable and for which, even in their absence, a nontrivial matching of solutions across the boundary separating classically allowed and classically forbidden regions must be performed. While Maslov and others have developed elegant methods for dealing with these complications [25] their techniques are more appropriate in the short wavelength limit wherein wave packets of highly excited states are evolved for finite time intervals. On the other hand our approach is aimed at the ground and lower excited states though, in principle, it is not limited thereto.

As we have already mentioned though, our approach is a natural variation of one that has been extensively developed in the microlocal analysis literature but it also differs from this innovative work in fundamental ways that are crucial for our ultimate, intended application to field theoretic problems. In the microlocal approach [18, 19, 20] one begins by analyzing the (classical, inverted potential) dynamics locally, near an equilibrium, by appealing to the stable manifold theorem of mechanics [26]. One then shows, by a separate argument, that, for an equilibrium p (lying in some neighborhood $U \subset \mathbb{R}^n$) the corresponding stable ($W^s(p) \subset T^*U$) and unstable ($W^u(p) \subset T^*U$) submanifolds of the associated phase space T^*U are in fact Lagrangian submanifolds that can be characterized as graphs of the (positive and negative) gradients of a smooth function $\phi : U \to \mathbb{R}$:

$$W^s(p) = \{(\mathbf{x}, \mathbf{p}) | \mathbf{x} \in U, \mathbf{p} = \nabla\phi(\mathbf{x})\} \tag{78}$$

$$W^u(p) = \{(\mathbf{x}, \mathbf{p}) | \mathbf{x} \in U, \mathbf{p} = -\nabla\phi(\mathbf{x})\}\,. \tag{79}$$

This function is shown to satisfy a certain 'eikonal' equation (equivalent to our inverted-potential-vanishing-energy Hamilton-Jacobi equation restricted to U) and $\phi(\mathbf{x})$ itself is, of course, nothing but the (locally defined) analogue of our action function $\mathcal{S}_{(0)}(\mathbf{x})$. A further argument is then needed to extend $\phi(x)$ to a solution globally defined on $\mathbb{R}^n$.

The potential energies, $V(\mathbf{x})$, dealt with in the microlocal literature often entail multiple local minima, or "wells", for which our global convexity and coercivity hypotheses are not appropriate. Much of the detailed analysis therein involves a careful matching of locally defined approximate solutions (constructed on suitable neighborhoods of each well) to yield global asymptotic approximations to the eigenvalues and eigenfunctions for such problems. Since, however, we are focussed primarily on potential energies having

single wells (corresponding to unique classical "vacuum states"), many of the technical features of this elegant analysis are not directly relevant to the issues of interest herein.

For the case of a single well, however, we have essentially unified and globalized several of the, aforementioned, local arguments, replacing them with the integrated study of the properties of the (inverted potential) action functional (48). When one turns from finite dimensional problems to field theoretic ones [11, 12] this change of analytical strategy will be seen to play an absolutely crucial role. For the typical (relativistic, bosonic) field theories of interest to us in this context, the Euler Lagrange equations for the corresponding, inverted potential action functionals that now arise are the *Euclidean signature*, elliptic analogues of the Lorentzian signature, hyperbolic field equations that one is endeavoring to quantize. While generalizations of the aforementioned stable manifold theorem do exist for certain types of infinite dimensional dynamical systems, the elliptic field equations of interest to us do not correspond to well-defined dynamical systems *at all*. In particular their associated Cauchy initial value problems are never well-posed. This is the main reason, in our opinion, why the traditional microlocal methods have not heretofore been applicable to quantum field theories.

On the other hand the direct method of the calculus of variations is applicable to the Euclidean signature action functionals of interest to us here and allows one to generalize the principle arguments discussed above to a natural infinite dimensional setting.

3.2. Interacting scalar fields

For a first glimpse at how these techniques can be applied to relativistic quantum field theories consider the formal Schrödinger operator for the massive, quartically self-interacting scalar field on (3+1 dimensional) Minkowski spacetime given by

$$\hat{H} = \int_{\mathbb{R}^3} \left\{ -\frac{\hbar^2}{2} \frac{\delta^2}{\delta\phi^2(\mathbf{x})} + \frac{1}{2}\nabla\phi(\mathbf{x}) \cdot \nabla\phi(\mathbf{x}) + \frac{m^2}{2}\phi^2(\mathbf{x}) + \lambda\phi^4(\mathbf{x}) \right\} d^3x \tag{80}$$

where m and λ are constants > 0. Though the functional Laplacian term, in particular, requires regularization to be well-defined, the influence of this regularization will only be felt at the level of quantum 'loop' corrections and not for the 'tree level' determination of a fundamental solution, $\mathcal{S}_{(0)}[\phi(\cdot)]$, to the

'vanishing-energy-Euclidean-signature' functional Hamilton-Jacobi equation given by

$$\int_{\mathbb{R}^3} \left\{ \frac{1}{2} \frac{\delta \mathcal{S}_{(0)}}{\delta \phi(\mathbf{x})} \frac{\delta \mathcal{S}_{(0)}}{\delta \phi(\mathbf{x})} - \frac{1}{2} \nabla \phi(\mathbf{x}) \cdot \nabla \phi(\mathbf{x}) - \frac{m^2}{2} \phi^2(\mathbf{x}) - \lambda \phi^4(\mathbf{x}) \right\} d^3x = 0. \tag{81}$$

As in the quantum mechanical examples discussed above this equation arises, at leading order, from substituting the ground state wave functional ansatz

$$\overset{(0)}{\Psi}_{\hbar}[\phi(\cdot)] = N_{\hbar} e^{-\mathcal{S}_{\hbar}[\phi(\cdot)]/\hbar} \tag{82}$$

into the time-independent Schrödinger equation

$$\hat{H} \overset{(0)}{\Psi}_{\hbar} = \overset{(0)}{E}_{\hbar} \overset{(0)}{\Psi}_{\hbar}, \tag{83}$$

and demanding satisfaction, order-by-order in powers of $\hbar$, relative to the formal expansions

$$\mathcal{S}_{\hbar}[\phi(\cdot)] \simeq \mathcal{S}_{(0)}[\phi(\cdot)] + \hbar \mathcal{S}_{(1)}[\phi(\cdot)] + \frac{\hbar^2}{2!} \mathcal{S}_{(2)}[\phi(\cdot)] + \cdots \tag{84}$$

and

$$\overset{(0)}{E}_{\hbar} \simeq \hbar \left\{ \overset{(0)}{\mathcal{E}}_{(0)} + \hbar \overset{(0)}{\mathcal{E}}_{(1)} + \frac{\hbar^2}{2!} \overset{(0)}{\mathcal{E}}_{(2)} + \cdots \right\}. \tag{85}$$

In the foregoing formulas $\phi(\cdot)$ symbolizes a real-valued distribution on $\mathbb{R}^3$ belonging to a certain Sobolev 'trace' space that we shall characterize more precisely below. In accordance with our strategy for solving the functional Hamilton-Jacobi equation (81) each such $\phi(\cdot)$ will be taken to represent boundary data, induced on the $t = 0$ hypersurface of (Euclidean)

$$\mathbb{R}^4 = \left\{ (t, \mathbf{x}) | t \in \mathbb{R}, \mathbf{x} \in \mathbb{R}^3 \right\}, \tag{86}$$

by a real (distributional) scalar field Φ defined on the half-space $\mathbb{R}^{4-} := (-\infty, 0] \times \mathbb{R}^3$. Here Φ plays the role of the curve $\gamma : (-\infty, 0] \to \mathbb{R}^n$ in

the quantum mechanics problem and $\phi(\cdot)$ the role of its right end point $(x^1, \ldots, x^n)$.

By generalizing the technique sketched above for the quantum mechanical problems the authors have proven the existence of a (globally-defined, Fréchet smooth) 'fundamental solution', $\mathcal{S}_{(0)}[\phi(\cdot)]$ to Eq. (81) by first establishing the existence of unique minimizers, Φ_ϕ, for the Euclidean-signature action functional

$$\mathcal{I}_{es}[\Phi] := \int_{\mathbb{R}^3} \int_{-\infty}^{0} \left\{ \frac{1}{2}\dot{\Phi}^2 + \frac{1}{2}\nabla\Phi \cdot \nabla\Phi + \frac{1}{2}m^2\Phi^2 + \lambda\Phi^4 \right\} dt\, d^3x \tag{87}$$

for 'arbitrary' boundary data $\phi(\cdot)$, prescribed at $t = 0$ and then setting

$$\mathcal{S}_{(0)}[\phi(\cdot)] = \mathcal{I}_{es}[\Phi_\phi]. \tag{88}$$

This was accomplished by defining the action functional $\mathcal{I}_{es}[\Phi]$ on the Sobolev space $H^1(\mathbb{R}^{4-}, \mathbb{R})$, with boundary data naturally induced on the corresponding trace space, and proving that this functional is coercive, weakly (sequentially) lower semi-continuous and convex [11]. Through an application of the (Banach space) implicit function theorem we then proved that the functional so-defined is Fréchet smooth throughout its (Sobolev trace space) domain of definition and that it indeed satisfies the (Eucliedean-signature-vanishing-energy) functional Hamilton-Jacobi equation,

$$\frac{1}{2}\int_{\mathbb{R}^3} \left| \frac{\delta \mathcal{S}_{(0)}[\phi(\cdot)]}{\delta\phi(\mathbf{x})} \right|^2 d^3x = \int_{\mathbb{R}^3} \left\{ \frac{1}{2}\nabla\phi(\mathbf{x}) \cdot \nabla\phi(\mathbf{x}) + \frac{1}{2}m^2\, \phi^2(\mathbf{x}) + \lambda\phi^4(\mathbf{x}) \right\} d^3x, \tag{89}$$

and thus provides the fundamental solution that one needs for the computation of all higher order quantum 'loop' corrections. These analytical methods were shown to work equally well in lower spatial dimensions for certain higher-order nonlinearities, allowing, for example, Φ^6 in (Euclidean) $\mathbb{R}^{3-}$ and Φ^p for any even $p > 2$ in $\mathbb{R}^{2-}$, and also for more general convex polynomial interaction potentials $\mathcal{P}(\Phi)$, allowing terms of intermediate degrees, replacing the $\frac{1}{2}m^2\Phi^2 + \lambda\Phi^4$ of the example above. These correspond precisely to the usual 'renormalizable' cases when treated by more conventional quantization methods. For us the restriction on the allowed

polynomial degree in a given spacetime dimension results from applying the Sobolev embedding theorem,

$$H^1(\mathbb{R}^- \times \mathbb{R}^n) \hookrightarrow L^p(\mathbb{R}^- \times \mathbb{R}^n) \tag{90}$$

for $2 \leq p \leq 2(n+1)/(n-1)$ if $n > 1$ and for any $p \geq 2$ if $n = 1$ (noting here that the domain in question has dimension $n + 1$), to the demand (needed in our analysis) that the higher order terms in the corresponding action functional be bounded by (some power of) the $H^1(\mathbb{R}^- \times \mathbb{R}^n)$ norm defined by the quadratic terms.

To compute higher order 'loop' corrections in this field theoretic setting one will first need to regularize the formal functional Laplacian that arises in the Schrödinger operator (80) and that will reoccur in each of the transport equations that result from substituting ansätze such as (82), (84) and (85) into the time independent Schrödinger equation (83) and requiring satisfaction order-by-order in powers of $\hbar$. Solving these transport equations for the 'loop corrections', $\{\mathcal{S}_{(1)}[\varphi(\cdot)], \mathcal{S}_{(2)}[\varphi(\cdot)], \ldots\}$, to the ground state wave functional simply amounts to *evaluating* sequentially computable, smooth functionals on the Euclidean signature action minimizers, Φ_ϕ, for arbitrarily chosen boundary data $\varphi(\cdot)$.

Solving the transport equations for excited states is somewhat more involved since these equations entail a lower order term in the unknown but the technology for handling this (at least in finite dimensions) is well-understood [10, 18, 19]. If, in particular, a Sternberg diffeomorphism could be shown to exist for field theoretic problems of the type discussed herein then the leading order, excited state transport equation could be solved in closed form. Otherwise though one could simply fall back on the machinery developed in Refs. [10, 18, 19], which does not assume the existence of Sternberg coordinates, and solve this and the corresponding higher order excited state equations in a less direct fashion since the aforementioned 'machinery' apparently generalizes, in a straightforward way, to this infinite dimensional setting. In either case it is intriguing to note that the excited states for *interacting* field theories would be naturally labeled by sequences of (integral) 'particle excitation numbers' in much the same way that the Fock-space excited states of a free field are characterized.

Indeed, modulo some apparently quite modest technicalities, needed to handle a continuous range of frequencies, it seems clear that when these same (Euclidean-signature-semi-classical) methods are applied to *free*, bosonic field theories they will simply regenerate the well-known (Fock-space) exact solutions for these systems. In particular the fundamental solutions to

the relevant (Euclidean signature) Hamilton-Jacobi equations are explicitly known for the most interesting cases ([27], and from a different perspective [28]), the higher order 'loop corrections' $\{\mathcal{S}_{(1)}[\varphi(\cdot)], \mathcal{S}_{(2)}[\varphi(\cdot)], \ldots\}$ will be found all to vanish (as they do for finite dimensional, *harmonic* oscillators) and the natural coordinates on the configuration manifold (i.e., the associated trace space described above) are already of Sternberg type.

One often hears that the fundamental particle interpretation of *interacting* quantized fields hinges upon their approximation, asymptotically, by corresponding *free* fields. This is somewhat unsatisfactory since, of course, an elementary particle cannot 'turn off' its self-interactions to behave, even asymptotically, like a Fock-space, free field quantum. While we do not yet have a clear 'physical interpretation' of the integral, 'excitation numbers' that would label our excited states one of the natural features of this (Euclidean-signature-semi-classical) program is that it maintains the dynamical nonlinearities of an interacting quantum system intact at every level of the analysis rather than attempting to reinstate nonlinear effects gradually through a perturbative expansion. One of our main motivations for pursuing it is the expectation that it will ultimately provide much more accurate approximations for wave functionals and their associated, *non-gaussian* integration measures than those generated by conventional (Rayleigh/Schrödinger) perturbation theory.

3.3. Yang-Mills fields

In continuing research the authors are currently applying these (Euclidean-signature-semi-classical) techniques to the quantization of Yang-Mills fields [12]. While the methods in question apply equally well to both 3 and 4 dimensional gauge theories (i.e., to the renormalizable cases), we shall focus here on the physically most interesting case of Yang-Mills fields in 4 spacetime dimensions. The formal Schrödinger operator for this system is expressible as

$$\hat{H}_{YM} := \int_{\mathbb{R}^3} \Sigma_I \left\{ -\frac{\hbar^2}{2} \sum_{i=1}^{3} \frac{\delta}{\delta A_i^I(\mathbf{x})} \frac{\delta}{\delta A_i^I(\mathbf{x})} + \frac{1}{4} \sum_{j,k=1}^{3} F_{jk}^I F_{jk}^I(\mathbf{x}) \right\} d^3x \tag{91}$$

where the index I labels a suitable basis for the Lie algebra of the gauge structure group G, A^I_k is the spatial connection field with curvature

$$F^I_{jk} = \partial_j A^I_k - \partial_k A^I_j + q[A_j, A_k]^I, \tag{92}$$

q is the gauge coupling constant and $[\cdot,\cdot]$ the bracket in the Lie algebra of the structure group G (under a matrix representation, the commutator).

As in the case of scalar field theory the functional Laplacian requires regularization to be well-defined even when acting on smooth functionals of the (spatial) connection but, since the influence of this regularization will not be felt until higher order quantum 'loop' corrections are computed, we can temporarily ignore this refinement here and attempt first to construct a (gauge invariant) fundamental solution, $\mathcal{S}_{(0)}[A(\cdot)]$, to the Euclidean-signature-vanishing-energy Hamilton-Jacobi equation

$$\int_{\mathbb{R}^3} \Sigma_i \left\{ \frac{1}{2} \sum_{i=1}^{3} \frac{\delta \mathcal{S}_{(0)}}{\delta A^I_i(\mathbf{x})} \frac{\delta \mathcal{S}_{(0)}}{\delta A^I_i(\mathbf{x})} - \frac{1}{4} \sum_{j,k=1}^{3} F^I_{jk}(\mathbf{x}) F^I_{jk}(\mathbf{x}) \right\} d^3x = 0 \tag{93}$$

by seeking minimizers of the corresponding Euclidean-signature action functional in the form of (spacetime) connections $\{\mathcal{A}^I_\mu\}$ defined on $\mathbb{R}^{4-} = (-\infty, 0] \times \mathbb{R}^3$ with boundary data A^I_i prescribed at $t = 0$.

As usual in our approach, Eq. (93) results from substituting the ansätze

$$\overset{(0)}{\Psi}_\hbar[A(\cdot)] = N_\hbar e^{-\mathcal{S}_\hbar[A(\cdot)]/\hbar}, \tag{94}$$

$$\mathcal{S}_\hbar[A(\cdot)] \simeq \mathcal{S}_{(0)}[A(\cdot)] + \hbar \mathcal{S}_{(1)}[A(\cdot)] + \frac{\hbar^2}{2!} \mathcal{S}_{(2)}[A(\cdot)] + \cdots + \frac{\hbar^k}{k!} \mathcal{S}_{(k)}[A(\cdot)] + \cdots, \tag{95}$$

$$\overset{(0)}{E}_\hbar \simeq \hbar \left(\overset{(0)}{\mathcal{E}}_{(0)} + \hbar \overset{(0)}{\mathcal{E}}_{(1)} + \frac{\hbar^2}{2!} \overset{(0)}{\mathcal{E}}_{(2)} + \cdots + \frac{\hbar^k}{k!} \overset{(0)}{\mathcal{E}}_{(k)} + \cdots \right) \tag{96}$$

into the Schrödinger equation

$$\hat{H}_{YM} \overset{(0)}{\Psi}_{\hbar} = \overset{(0)}{E}_{\hbar} \overset{(0)}{\Psi}_{\hbar} \tag{97}$$

and demanding satisfaction order by order in $\hbar$.

To construct the functional $\mathcal{S}_{(0)}[A(\cdot)]$ we treat the (spatial) connection field $A = \{A_i^I\}$ on $\mathbb{R}^3$ as (tangential) boundary data for the Euclidean-signature Yang-Mills Dirichlet problem — prescribing this data on the hypersurface $\{x^0 = ct = 0\}$ of $\mathbb{R}^4 = \{(x^\mu) = (ct, \mathbf{x}) : \mathbf{x} = (x^1, x^2, x^3)\}$. Thus for 'arbitrary' boundary data A defined on $\{0\} \times \mathbb{R}^3$ (and lying in a suitable 'trace space' for spacetime connection fields $\mathcal{A} = \{\mathcal{A}_\mu^I\}$), we seek an absolute minimizer, $\mathcal{A}_A$, for the Euclidean-signature Yang-Mills action functional, $\mathcal{I}_{es}[\mathcal{A}]$, defined on the half-space $\mathbb{R}^- \times \mathbb{R}^3 := (-\infty, 0] \times \mathbb{R}^3$ by

$$\begin{aligned} \mathcal{I}_{es}[\mathcal{A}] &:= \frac{1}{4} \int_{\mathbb{R}^- \times \mathbb{R}^3} \left\{ \Sigma_I \sum_{\mu,\nu=0}^{3} [\mathcal{F}_{\mu\nu}^I \mathcal{F}_{\mu\nu}^I] \right\} dt\, d^3x \\ &= \frac{1}{2} \int_{-\infty}^{0} dt \int_{\mathbb{R}^3} d^3x \left\{ \Sigma_I \left[\sum_{i=1}^{3} (\partial_0 \mathcal{A}_i^I - \partial_i \mathcal{A}_0^I)^2 \right.\right. \\ &\quad \left.\left. + \frac{1}{2} \sum_{j,k=1}^{3} \mathcal{F}_{jk}^I \mathcal{F}_{jk}^I \right] \right\} \end{aligned} \tag{98}$$

where $\mathcal{F} = \{\mathcal{F}_{\mu\nu}^I\}$, the curvature of the connection $\mathcal{A}$, is given by

$$\mathcal{F}_{\mu\nu}^I := \partial_\mu \mathcal{A}_\nu^I - \partial_\nu \mathcal{A}_\mu^I + q[\mathcal{A}_\mu, \mathcal{A}_\nu]^I. \tag{99}$$

The first question our construction must address is that of defining the function space from which Yang-Mills connections on $\{0\} \times \mathbb{R}^3$ (viewed as initial data for the Euclidean-signature Dirichlet problem on the half-space $\mathbb{R}^{4-}$) are to be drawn. Modulo the action of gauge transformations, this function space of connections yields as its quotient the orbit space which is the true Yang-Mills configuration space.

In particular, our construction proceeds differently depending on whether or not we require each connection to approach a coherent value at spatial infinity, as done for instance by Jackiw in [29]. Under this requirement, the initial hypersurface $\{0\} \times \mathbb{R}^3$ effectively becomes a 3-sphere, introducing a distinction between 'small' and 'large' gauge transformations

(homotopically trivial and nontrivial, respectively), and an attendant division of the Yang-Mills configuration space into distinct topological sectors. The dichotomy between large and small gauge transformations is usually seen as the origin of the 'vacuum angle' in quantum Yang-Mills theory, with wave functionals invariant only up to a phase under large gauge transformations [29]. As in the treatment by Khoze [30], we allow connections to have no coherent limit at spatial infinity, and regard all gauge transformations on the same footing. Nevertheless our approach, like others with the same definition of the configuration space, is not incompatible with the introduction of a vacuum angle, since such a feature (if present in nature) can be incorporated in the Lagrangian as observed in [29] and [30].

To prove existence of a minimizer for the Euclidean-signature Yang-Mills action with (tangential) initial data A prescribed from our configuration space on $\{0\} \times \mathbb{R}^3$, we use the direct method in the calculus of variations to conclude that any action-minimizing sequence with given initial data has a convergent subsequence, on whose limit the Euclidean-signature Yang-Mills action is indeed minimized. As in the physical models discussed in the preceding sections, we then define $\mathcal{S}_{(0)}[A(\cdot)]$ to assume the absolute minimizing value of the Euclidean-signature Yang-Mills action for initial data A.

The existence of a convergent minimizing subsequence is essentially due to weak compactness of bounded sets in Sobolev spaces. One is enabled to invoke Sobolev weak compactness by gauge transforming to a 'Hodge' or 'Coulomb' gauge locally on neighborhoods of $\mathbb{R}^{4-}$ where the curvature of connections in the minimizing sequence has sufficiently small L^2 norm. On such neighborhoods, a pivotal result of Uhlenbeck [31] states that one can transform to the Hodge gauge, and that the L^2_1 Sobolev norm of the transformed connection is bounded in terms of the L^2 norm of its curvature. Additionally, use of the (local) Hodge gauge allows the top order term in the Yang-Mills equation to be viewed as a Laplace-de Rham operator, making available elliptic regularity results to establish smoothness of the solution. For further details, the reader is referred to the work of Sedlacek [32] for a compact manifold without boundary, Marini [33] for a compact manifold with boundary, and the present authors [27, 12] for a possibly noncompact manifold with boundary.

While the local Hodge gauge is key to achieving existence and regularity of a minimizer, it should be noted that this method is internal to the proof and thence the construction of $\mathcal{S}_{(0)}$. Thus it does not introduce a Gribov ambiguity since it does not constitute a global gauge fixing within the Yang-Mills configuration space. We treat the domain of $\mathcal{S}_{(0)}$ as a Sobolev

space of connections, noting that gauge invariance of the Euclidean-signature Yang-Mills action immediately implies that $\mathcal{S}_{(0)}[A(\cdot)]$ is a (*fully non-Abelian*) gauge invariant solution to the Hamilton-Jacobi equation (93) and accordingly satisfies the corresponding Gauss-law constraint — namely the vanishing of the gauge covariant divergence of its (electric field) functional gradient, $\frac{\delta \mathcal{S}_{(0)}}{\delta A^I(\mathbf{x})}[A(\cdot)]$. As such $\mathcal{S}_{(0)}[A(\cdot)]$ will naturally pass to the quotient, orbit space whereon it will correspondingly satisfy the *reduced* Hamilton-Jacobi equation for this (positively curved) infinite dimensional Riemannian manifold. In establishing smoothness results for $\mathcal{S}_{(0)}$, we use the Sobolev topology on the space of connections which form its domain, employing the Banach space version of Rademacher's theorem to show that $\mathcal{S}_{(0)}$ is Gâteaux differentiable almost everywhere in a suitable sense (for details, see [12]). Application of the Banach space implicit function theorem to establish Fréchet differentiability of $\mathcal{S}_{(0)}$ to all orders is the topic of current investigations.

The self-interactions of 'gluons' (the quanta of the Yang-Mills field) are closely connected to the non-Abelian character of the associated gauge group. Thus a conventional perturbative approach to quantization, which disregards these interactions at the lowest order, necessarily 'approximates' the gauge group as well, replacing it with the Abelian structure group of the associated free field theory (i.e., several copies of the Maxwell field labelled by the index I), and then attempts to reinstate both the interactions and the non-commutative character of the actual gauge group gradually, through the development of series expansions in the Yang-Mills coupling constant. By contrast the Euclidean-signature-semi-classical program that we are advocating for the Yang-Mills problem has the advantage of maintaining *full, non-Abelian gauge invariance* at every order of the calculation and of generating globally defined (approximate) wave functionals on the naturally associated Yang-Mills configuration manifold.

4. The orbit space curvature for scalar electrodynamics

The Lagrangian density for 'scalar electrodynamics', as we shall use the term herein, is given by

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \eta^{\mu\nu}(D_\mu\varphi)^\dagger(D_\nu\varphi) - \mathcal{U}(\varphi^\dagger\varphi) \tag{100}$$

where $\varphi := \varphi^1 + i\varphi^2$, with φ^a real, is a complex scalar field, $\varphi^\dagger := \varphi^1 - i\varphi^2$ its complex conjugate and where $F = F_{\mu\nu}\, dx^\mu \otimes dx^\nu$ is the electromagnetic field

tensor expressible in terms of its associated connection or 'vector potential' $A = A_\mu dx^\mu$ as

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{101}$$

The gauge covariant derivatives $D_\mu\varphi$, $(D_\mu\varphi)^\dagger$ are defined by

$$D_\mu\varphi = \partial_\mu\varphi - iqA_\mu\varphi \tag{102}$$

$$(D_\mu\varphi)^\dagger = \partial_\mu\varphi^\dagger + iqA_\mu\varphi^\dagger \tag{103}$$

wherein q is a gauge 'coupling' constant having the dimensions

$$[q] = \left[\frac{e}{\hbar c}\right] \tag{104}$$

with e the fundamental constant of electric charge, $\hbar$ the (reduced) Planck constant and c the speed of light. The self-interaction potential $\mathcal{U} : \mathbb{R} \to \mathbb{R}$ is assumed to be smooth and positive. In the standard (Lorentz frame) coordinates, $\{x^\mu; \mu = 0, 1, 2, 3\} = \{ct, x^i; i = 1, 2, 3\}$, that we shall use the Minbowski metric $\eta = \eta_{\mu\nu} dx^\mu \otimes dx^\nu$ takes the form

$$\eta = -c^2 dt \otimes dt + \sum_{i=1}^{3} dx^i \otimes dx^i \tag{105}$$

with corresponding line element

$$ds^2 = -c^2 dt^2 + d\mathbf{x} \cdot d\mathbf{x} \tag{106}$$

where $\mathbf{x} := (x^1, x^2, x^3)$ and $\cdot$ designates the Euclidean metric on $\mathbb{R}^3$.

As is well-known $\mathcal{L}$ is invariant with respect to the group $\mathcal{G}$ of 'gauge transformations' under which

$$A_\mu \to A_\mu + \partial_\mu\Lambda, \qquad \varphi \to \varphi e^{iq\Lambda} \tag{107}$$

where Λ is an arbitrary, smooth function having the dimensions of 'charge', $[e]$, and vanishing at infinity, $|\mathbf{x}| := \sqrt{\mathbf{x} \cdot \mathbf{x}} \to \infty$. The action functional defined on any domain of the form $\Omega = I \times \mathbb{R}^3$, with $I = [t_0, t_1] \subset \mathbb{R}$, is given by

$$\mathcal{I}_\Omega[\varphi, A] := \frac{1}{c} \int_\Omega d^4x \; \mathcal{L} = \int_I dt \; L \tag{108}$$

where L is the Lagrangian defined by

$$L := \int_{\mathbb{R}^3} d^3x \, \mathcal{L}. \tag{109}$$

The Euler-Lagrange equations (for the domain Ω) obtained by varying $\mathcal{I}_\Omega[\varphi, A]$ with respect to φ and A are given (respectively) by

$$\eta^{\mu\nu} D_\mu D_\nu \varphi - \mathcal{U}'(\varphi^\dagger \varphi)\varphi = 0 \tag{110}$$

and

$$\partial_\nu F^{\mu\nu} = iq\eta^{\mu\nu} \left[(D_\nu \varphi)^\dagger \varphi - \varphi^\dagger (D_\nu \varphi) \right] \tag{111}$$

wherein $\mathcal{U}'(u) := \frac{d\mathcal{U}(u)}{du}$.

The time component, $\mu \to 0$, of the Maxwell equation (111) gives, of course, the Gauss law 'constraint'

$$\begin{aligned} \partial_i F^{0i} &= -\partial_i F_{0i} \\ &= -iq \left[(D_0 \varphi)^\dagger \varphi - \varphi^\dagger (D_0 \varphi) \right] \end{aligned} \tag{112}$$

which, expressed in terms of the vector potential A, becomes

$$-\Delta A_0 + 2q^2 \varphi^\dagger \varphi A_0 = -\partial_i (A_{i,0}) + iq \left[(\partial_0 \varphi^\dagger)\varphi - \varphi^\dagger (\partial_0 \varphi) \right] \tag{113}$$

with Δ the Laplacian on (Euclidean) $\mathbb{R}^3$,

$$\Delta = \sum_{i=1}^{3} \frac{\partial^2}{\partial x^{i2}}, \tag{114}$$

and where, in the above, we have adopted the summation convention for sums over repeated *spatial* indices (writing, e.g., $\partial_i v^i$ for $\sum_{i=1}^3 \partial_i v^i$).

The operator Δ_φ defined by

$$\Delta_\varphi := \Delta - 2q^2 \varphi^\dagger \varphi \tag{115}$$

will play a fundamental role in the following. In a suitable function space setting its inverse, Δ_φ^{-1}, will exist and allow one to solve the elliptic, Gauss law constraint for A_0 by setting

$$A_0 = \Delta_\varphi^{-1} \left[(\partial_i A_{i,0}) - iq \left[(\partial_0 \varphi^\dagger)\varphi - \varphi^\dagger (\partial_0 \varphi) \right] \right]. \tag{116}$$

Reexpressed in this 3+1 dimensional notation the Lagrangian defined above now takes the form

(117)
$$L = \int_{\mathbb{R}^3} d^3x \left\{ \frac{1}{2} F_{0j} F_{0j} - \frac{1}{4} F_{jk} F_{jk} + (D_0\varphi)^\dagger (D_0\varphi) - (D_j\varphi)^\dagger (D_j\varphi) - U(\varphi^\dagger\varphi) \right\}.$$

Defining canonical momenta π_φ and π^j conjugate to ∂ and A_j (respectively) by the Legendre transformation

$$\pi_\varphi := \frac{\delta L}{\delta \varphi_{,t}} = \frac{1}{c}(D_0\varphi)^\dagger \tag{118}$$

$$\pi^j := \frac{\delta L}{\delta A_{j,t}} = \frac{1}{c}(A_{j,0} - A_{0,j}) = \frac{1}{c} F_{0j} \tag{119}$$

with, of course,

$$\pi^\dagger_\varphi := \frac{\delta L}{\delta \varphi^\dagger_{,t}} = \frac{1}{c}(D_0\varphi) \tag{120}$$

and noting that

$$\pi^0 := \frac{\delta L}{\delta A_{0,t}} \equiv 0 \tag{121}$$

one arrives at the associated Hamiltonian density

$$\mathcal{H} := \pi_\varphi \varphi_{,t} + \pi_{\varphi^\dagger} \varphi^\dagger_{,t} + \pi^j A_{j,t} - \mathcal{L}. \tag{122}$$

The corresponding Hamiltonian takes the explicit form

(123)
$$\begin{aligned} H &:= \int_{\mathbb{R}^3} dx^3 \mathcal{H} \\ &= \int_{\mathbb{R}^3} d^3x \left\{ \frac{1}{2} c^2 \pi^j \pi^j + c^2 \pi^\dagger_\varphi \pi_\varphi + \frac{1}{4} F_{jk} F_{jk} + (D_j\varphi)^\dagger (D_j\varphi) + U(\varphi^\dagger\varphi) \right. \\ &\quad \left. - A_0 \left[\partial_j (c\pi^j) - iqc(\varphi\pi_\varphi - \varphi^\dagger \pi^\dagger_\varphi) \right] \right\} \\ &\quad + \int_{\mathbb{R}^3} d^3x (\partial_j \left(A_0 c \pi^j \right)) \end{aligned}$$

wherein A_0 now plays the role of a 'Lagrange multiplier' with respect to whose variation one recovers the Hamiltonian form of the Gauss constraint

$$\partial_j(c\pi^j) = iq\left(\varphi(c\pi_\varphi) - \varphi^\dagger(c\pi_\varphi^\dagger)\right). \tag{124}$$

Noting that $c\pi^j = F_{0j} = -E^j$, where $\mathbf{E} = E^j \frac{\partial}{\partial x_j}$ is the electric field, one sees that the (gauge invariant) charge density ρ of the φ field is given by

$$\begin{aligned} 4\pi\rho &= -iq\left(\varphi(c\pi_\varphi) - \varphi^\dagger(c\pi_\varphi^\dagger)\right) \\ &= -iq\left(\varphi(D_0\varphi)^\dagger - \varphi^\dagger(D_0\varphi)\right). \end{aligned} \tag{125}$$

Again in a suitable function space setting one can decompose $\boldsymbol{\pi} = \pi^j \frac{\partial}{\partial x^j}$ into L^2-orthogonal 'transverse' and 'longitudinal' components,

$$\boldsymbol{\pi} = \boldsymbol{\pi}^T + \boldsymbol{\pi}^L, \tag{126}$$

with

$$\nabla \cdot \boldsymbol{\pi}^T = \partial_j(\pi^T)^j = 0, \tag{127}$$

$$\boldsymbol{\pi}^L = \nabla\lambda \tag{128}$$

so that

$$\nabla \cdot \boldsymbol{\pi} = \nabla \cdot \boldsymbol{\pi}^L = \Delta\lambda \tag{129}$$

and thereby express the solution of the Gauss constraint in the (Hamiltonian) form

$$\begin{aligned} -(c\boldsymbol{\pi}^L)^j &:= (\mathbf{E}^L)^j \\ &= -\nabla^j\left(\Delta^{-1}\left[iq\left(\varphi(c\pi_\varphi) - \varphi^\dagger(c\pi_\varphi^\dagger)\right)\right]\right) \\ &= \nabla^j\left(\Delta^{-1}(4\pi\rho)\right) \end{aligned} \tag{130}$$

where, more explicitly,

$$\left(\Delta^{-1}(4\pi\rho)\right)(\mathbf{x}) = -\int_{\mathbb{R}^3} d^3x' \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \tag{131}$$

with $|\mathbf{x} - \mathbf{x}'|$ the Euclidean distance from $\mathbf{x}$ to $\mathbf{x}'$.

In parallel with the above decomposition of $\boldsymbol{\pi}$, we can also express A_i in terms of L^2-orthogonal transverse and longitudinal summands via

$$A_i = A_i^T + A_i^L \tag{132}$$

with

$$\nabla \cdot \mathbf{A}^T = \partial_j A_j^T = 0 \tag{133}$$

and

$$\nabla \times \mathbf{A}^L = 0 \tag{134}$$

with $\mathbf{A}^L$ given explicitly by

$$A_j^L(\mathbf{x}) = -\partial_j \left[\int_{\mathbb{R}^3} d^3x' \left(\frac{(\partial_k A_k(\mathbf{x}'))}{4\pi|\mathbf{x}-\mathbf{x}'|} \right) \right]. \tag{135}$$

Note accordingly that one can always achieve the 'Coulomb gauge' condition $\mathbf{A}^L = 0$ with the $\mathcal{G}$ action generated by

$$\Lambda(\mathbf{x}) = \int_{\mathbb{R}^3} d^3x' \left(\frac{\partial_k A_k(\mathbf{x}')}{4\pi|\mathbf{x}-\mathbf{x}'|} \right) \tag{136}$$

under which φ undergoes the corresponding change of 'phase' $\varphi \to \varphi e^{iq\Lambda}$. In an arbitrary gauge it is easily verified that $\{\mathbf{A}^T, \boldsymbol{\pi}^T\}$ and $\{\mathbf{A}^L, \boldsymbol{\pi}^L\}$ are canonically conjugate variables. Since $\boldsymbol{\pi}^L$ is uniquely determined by the charge density however (cf. 130) and since its conjugate partner can be eliminated by the choice of Coulomb gauge it is natural to pass to a *reduced Hamiltonian* framework.

We therefore define a 'reduced' Hamiltonian by substituting the above expression (130) for $\boldsymbol{\pi}^L$ into H, dropping the boundary integral, $\int_{\mathbb{R}^3} d^3x \left(\partial_j (A_0 c\pi^j)\right)$, (which makes no contribution to the field equations) and imposing the Coulomb gauge condition under which $A_j \to A_j^T$. The result is

$$\begin{aligned} H_{\text{reduced}} := \int_{\mathbb{R}^3} d^3x \Big\{ & \frac{1}{2} c^2 \boldsymbol{\pi}^T \cdot \boldsymbol{\pi}^T + c^2 \pi_\varphi^\dagger \pi_\varphi + \frac{1}{4} F_{jk} F_{jk} \\ & + (D_j\varphi)^\dagger (D_j\varphi) + U(\varphi^\dagger\varphi) \\ & + \frac{1}{2} q^2 c^2 (\varphi\pi_\varphi - \varphi^\dagger \pi_\varphi^\dagger) \Delta^{-1} (\varphi\pi_\varphi - \varphi^\dagger \pi_\varphi^\dagger) \Big\} \end{aligned} \tag{137}$$

wherein

$$\left(\Delta^{-1}(\varphi\pi_\varphi - \varphi^\dagger\pi_\varphi^\dagger)\right)(\mathbf{x}) = -\frac{1}{4\pi}\int_{\mathbb{R}^3} d^3x' \left(\frac{(\varphi\pi_\varphi - \varphi^\dagger\pi_\varphi^\dagger)(\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|}\right). \tag{138}$$

Note that, in this gauge, Eq. (116) for A_0 simplifies to

$$A_0 = \Delta_\varphi^{-1}\left[-iq\left[(\partial_0\varphi^\dagger)\varphi - \varphi^\dagger(\partial_0\varphi)\right]\right] \tag{139}$$

or, since

$$\Delta_\varphi A_0 = -iq\left[(\partial_0\varphi^\dagger)\varphi - \varphi^\dagger(\partial_0\varphi)\right] \tag{140}$$

can be expressed as

$$\Delta A_0 = -iq\left[(c\pi_\varphi)\varphi - (c\pi_\varphi^\dagger)\varphi^\dagger\right], \tag{141}$$

also to

$$A_0 = \Delta^{-1}\left[-iq\left[(c\pi_\varphi)\varphi - (c\pi_\varphi^\dagger)\varphi^\dagger\right]\right]. \tag{142}$$

The reduced Lagrangian that corresponds to H_{reduced} may be equivalently derived by substituting (139) and $\mathbf{A}^L = 0$ into L or by inverting the Legendre transformation determined by H_{reduced}. The result is:

$$\begin{aligned} L_{\text{reduced}} := \int_{\mathbb{R}^3} d^3x \Big\{ & \frac{1}{2c^2}\mathbf{A}^T_{,t}\cdot\mathbf{A}^T_{,t} + \frac{1}{c^2}(\varphi^\dagger_{,t})(\varphi_{,t}) \\ & - \frac{1}{4}F_{jk}F_{jk} - (D_j\varphi)^\dagger(D_j\varphi) - U(\varphi^\dagger\varphi) \\ & - \frac{q^2}{2c^2}(\varphi^\dagger_{,t}\varphi - \varphi_{,t}\varphi^\dagger)\Delta_\varphi^{-1}(\varphi^\dagger_{,t}\varphi - \varphi_{,t}\varphi^\dagger)\Big\} \end{aligned} \tag{143}$$

Prior to reduction the configuration manifold $\mathcal{Q}$ can be regarded as the product of the space of (spatial) connections $\mathcal{A}$ with the space of complex scalar fields $\mathcal{S}$, all defined over $\mathbb{R}^3$:

$$\mathcal{Q} = \mathcal{A}\times\mathcal{S} \tag{144}$$

The Hamiltonian H is defined on its associated cotangent bundle

$$\mathcal{P} = T^*\mathcal{Q} \tag{145}$$

but depends not only on the corresponding canonical variables but also on the (at this point still arbitrary) 'Lagrange multiplier' field A_0. The natural *reduced* configuration manifold, $\mathcal{Q}_{\text{reduced}}$, can be viewed as the abstract quotient of $\mathcal{Q}$ by the gauge group $\mathcal{G}$

$$\mathcal{Q}_{\text{reduced}} := \mathcal{Q}/\mathcal{G} \tag{146}$$

so that, in more geometric language, $\mathcal{Q}$ is a $\mathcal{G}$-bundle over $\mathcal{Q}_{\text{reduced}}$. By the same token the reduced phase space (over which H_{reduced} is defined) can be regarded as the cotangent bundle of $\mathcal{Q}_{\text{reduced}}$

$$\mathcal{P}_{\text{reduced}} := T^*\mathcal{Q}_{\text{reduced}}. \tag{147}$$

The Coulomb gauge condition defines a smooth, global cross-section of this (topologically trivial) bundle

$$\mathcal{Q} \to \mathcal{Q}_{\text{reduced}} = \mathcal{Q}/\mathcal{G} \tag{148}$$

and thus may be viewed as providing a concrete realization of this abstract quotient space in terms of an explicit submanifold of $\mathcal{Q}$. In this setting the reduced-space canonical variables $\{\mathbf{A}^T, \varphi\}$ effectively provide a global coordinate system for the quotient manifold, $\mathcal{Q}_{\text{reduced}}$, and, together with their conjugate momenta $\{\boldsymbol{\pi}^T, \pi_\varphi\}$, define global canonical coordinates for $\mathcal{P}_{\text{reduced}}$. A different choice of gauge up in the bundle (other than the Coulomb one that we have made) would have induced a different coordinate system down in the base without, however, modifying the (gauge) invariant dynamics unfolding in the quotient, 'orbit' space.

From the purely 'kinetic energy' terms in L_{reduced} (i.e., those bilinear in $\varphi_{,t}$ and $\varphi^\dagger_{,t}$) and in H_{reduced} (i.e., those bilinear in π_φ and $\pi^\dagger_\varphi$) one can read off coordinate expressions for the naturally induced (product) Riemannian metric, ${}^{\mathcal{Q}}\mathbf{g}$, defined on $\mathcal{Q}_{\text{reduced}}$ and its inverse, ${}^{\mathcal{Q}}\mathbf{g}^{-1}$. The metric in the $\mathcal{A}^T$ factor is manifestly 'Euclidean' whereas that on the $\mathcal{S}$ factor takes (in a notation explicitly geared to the chosen coordinate system) the form:

$$\mathbf{g}_{\varphi^a(\mathbf{x})\varphi^b(\mathbf{x}')} := \frac{2}{c^2}\left\{\delta_{ab}\delta(\mathbf{x},\mathbf{x}') + 2q^2\epsilon_{ac}\varphi^c(\mathbf{x})\Delta_\varphi^{-1}(\mathbf{x},\mathbf{x}')\epsilon_{bd}\varphi^d(\mathbf{x}')\right\} \tag{149}$$

where $\Delta_\varphi^{-1}(\mathbf{x},\mathbf{x}')$ is the kernel function for the operator Δ_φ^{-1} and where $\epsilon^{ab} = -\epsilon^{ba}$ with $\epsilon^{12} = 1$. The inverse (i.e., contra-variant) form of this metric is given by

$$\mathbf{g}^{\varphi^a(\mathbf{x})\varphi^b(\mathbf{x}')} := \frac{c^2}{2}\left\{\delta^{ab}\delta(\mathbf{x},\mathbf{x}') + 2q^2\frac{\epsilon^{ac}\varphi_c(\mathbf{x})\epsilon^{bd}\varphi_d(\mathbf{x}')}{4\pi|\mathbf{x}-\mathbf{x}'|}\right\} \tag{150}$$

with $\varphi_a = \delta_{ab}\varphi^b = \varphi^a$ and $\epsilon^{ab} = \epsilon_{ab}$. With these definitions the kinetic energy term, $\mathcal{K}_\varphi$, for the $\mathcal{S}$ factor can be written as

$$\mathcal{K}_\varphi = \frac{1}{2}\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3x' \left\{ \mathrm{g}_{\varphi^a(\mathbf{x})\varphi^b(\mathbf{x}')}\varphi^a_{,t}(\mathbf{x})\varphi^b_{,t}(\mathbf{x}') \right\} \tag{151}$$

or, equivalently, as

$$\mathcal{K}_\varphi = \frac{1}{2}\int_{\mathbb{R}^3} d^3x \int_{\mathbb{R}^3} d^3x' \left\{ \mathrm{g}^{\varphi^a(\mathbf{x})\varphi^b(\mathbf{x}')}\pi_a(\mathbf{x})\pi_b(\mathbf{x}') \right\} \tag{152}$$

where

$$\pi_1 := \pi_\varphi + \pi^\dagger_\varphi \tag{153}$$

and

$$\pi_2 := i(\pi_\varphi - \pi^\dagger_\varphi) \tag{154}$$

are the momenta conjugate to φ^1 and φ^2 (respectively) so that, in particular,

$$\pi_\varphi \varphi_{,t} + \pi^\dagger_\varphi \varphi^\dagger_{,t} = \pi_1\varphi^1_{,t} + \pi_2\varphi^2_{,t}. \tag{155}$$

Recalling that the kernel function, $\Delta^{-1}(\mathbf{x}, \mathbf{x}')$, for the operator Δ^{-1} is given by

$$\Delta^{-1}(\mathbf{x}, \mathbf{x}') = \frac{-1}{4\pi|\mathbf{x} - \mathbf{x}'|} \tag{156}$$

it is not difficult to verify directly that g and g^{-1} are indeed inverses of one another and hence satisfy

$$\int_{\mathbb{R}^3} d^3x' \left(\mathrm{g}_{\varphi^a(\mathbf{x})\varphi^b(\mathbf{x}')}\mathrm{g}^{\varphi^b(\mathbf{x}')\varphi^c(\mathbf{x}'')} \right) = \delta^c_a \delta(\mathbf{x}, \mathbf{x}''). \tag{157}$$

This identity plays a key role in the Legendre transformation relating L_{reduced} to H_{reduced}.

While it would now be straightforward to compute the curvature of the manifold $(\mathcal{S}, \mathrm{g})$ directly in the global chart defined above there is an alternative approach that allows for an easier comparison of the curvatures at different points of $\mathcal{S}$ as well as for an illuminating comparison with the corresponding results for Yang-Mills fields derived in [1, 2, 3]. This alternative

involves solving the geodesic equations for the manifold $(\mathcal{S}, \mathsf{g})$, constructing the exponential map associated to an *arbitrary point* of $\mathcal{S}$ and thereby introducing an analogue of *normal coordinates* centered at the chosen point. In normal coordinates the connection components vanish at the chosen point thereby dramatically simplifying the evaluation of the corresponding curvature at that point.

The reduced Hamilton equations for the φ field are readily found to be

$$\begin{aligned} \varphi_{,t} &= \frac{\delta H_{\text{reduced}}}{\delta \pi_\varphi} \\ &= c^2 \pi_\varphi^\dagger + iqcA_0\varphi \end{aligned} \tag{158}$$

and

$$\begin{aligned} (\pi_\varphi^\dagger)_{,t} &= -\frac{\delta H_{\text{reduced}}}{\delta \varphi^\dagger} \\ &= iqcA_0\pi_\varphi^\dagger - \frac{\delta}{\delta \varphi^\dagger} \int_{\mathbb{R}^3} d^3x \left\{ (D_j\varphi)^\dagger (D_j\varphi) + U(\varphi^\dagger\varphi) \right\} \end{aligned} \tag{159}$$

in which

$$A_0 = \Delta^{-1} \left[-iq(\varphi c\pi_\varphi - \varphi^\dagger c\pi_\varphi^\dagger) \right] \tag{160}$$

as was shown (in Eq. (142)) above. The geodesic equations result from simply dropping the 'forcing term' in the $(\pi_\varphi^\dagger)_{,t}$ equation and thus correspond to

$$\varphi_{,0} - iqA_0\varphi = c\pi_\varphi^\dagger = D_0\varphi \tag{161}$$

and

$$(c\pi_\varphi^\dagger)_{,0} - iqA_0(c\pi_\varphi^\dagger) = 0. \tag{162}$$

It follows immediately from differentiating Eq. (160) for A_0 that, *for the geodesics problem*,

$$A_{0,0} = 0 \qquad \text{(for geodesics)}. \tag{163}$$

Combining Eqs. (161), (162) and (163) one arrives at a second order form for the geodesic equations

$$\begin{aligned} D_0 D_0 \varphi &= \varphi_{,00} - 2iqA_0\varphi_{,0} - q^2 A_0^2 \varphi \\ &= 0. \end{aligned} \tag{164}$$

The general solution of this equation is expressible as

$$\varphi = (\alpha + \beta x^0) e^{iqA_0 x^0} \tag{165}$$

where α and β are 'arbitrary' complex fields independent of x^0. One easily finds that

$$\varphi(D_0\varphi)^\dagger - \varphi^\dagger(D_0\varphi) = \beta^\dagger\alpha - \beta\alpha^\dagger \tag{166}$$

so that A_0 becomes expressible as

$$\begin{aligned} iqA_0 &= q^2\Delta^{-1}\left[\varphi(D_0\varphi)^\dagger - \varphi^\dagger(D_0\varphi)\right] \\ &= q^2\Delta^{-1}(\beta^\dagger\alpha - \beta\alpha^\dagger) \end{aligned} \tag{167}$$

which explicitly displays its time independence.

For the exponential map however we want the geodesic expressed in terms of tangent space initial data $\{\varphi|_{x^0=0}, \varphi_{,0}|_{x^0=0}\}$ but, whereas $\varphi|_{x^0=0} = \alpha$, one finds that

$$\beta = \varphi_{,0}|_{x^0=0} - iqA_0\,\varphi|_{x^0=0} \tag{168}$$

which, in view of (167), is difficult to solve for β. Using the alternative expression for A_0 given by (139), however, one can write

$$\begin{aligned} iqA_0 &= \left\{q^2\Delta_\varphi^{-1}\left[\varphi(\partial_0\varphi^\dagger) - \varphi^\dagger(\partial_0\varphi)\right]\right\}\Big|_{x^0=0} \\ &= q^2\Delta_\alpha^{-1}[\alpha\zeta^\dagger - \alpha^\dagger\zeta] \end{aligned} \tag{169}$$

where $\zeta := \varphi_{,0}|_{x^0=0}$. Substituting these expressions into (165) yields the derived formula for geodesics expressed in terms of tangent space initial data $\{\alpha, \zeta\}$:

$$\varphi = \left(\alpha(1 - iqA_0x^0) + \zeta x^0\right) e^{iqA_0x^0}. \tag{170}$$

Evaluating this at a fixed 'unit of time' $x^0 = \ell^0 = ct^0$ and defining the

'normal' coordinate h by[9]

$$h := \ell^0 \zeta = \ell^0(\partial_0 \varphi)\big|_{x^0=0} \tag{171}$$

one arrives at our explicit formula for the exponential map

$$\varphi_h = \left\{ \alpha \left(1 - q^2 \Delta_\alpha^{-1}(\alpha h^\dagger - \alpha^\dagger h) \right) + h \right\} e^{q^2 \Delta_\alpha^{-1}[\alpha h^\dagger - \alpha^\dagger h]} \tag{172}$$

which for arbitrary fixed α, will be smoothly invertible on a sufficiently small 'normal' neighborhood of this chosen point which, of course, corresponds to the 'origin' $h = 0$.

To compute the metric g in normal coordinates we need only evaluate the kinetic energy term $\mathcal{K}_\varphi$ (cf. Eq. (151)) along an arbitrary differentiable curve (in the chosen chart for $\mathcal{S}$) after substituting φ_h for φ everywhere. To calculate the curvature tensor at the (arbitrary) reference point α, however, one only needs the transformed expression for g expanded out to second order in h. To this end note that

$$\begin{aligned} \Delta_{\varphi_h} &:= \Delta - 2q^2 \varphi_h^\dagger \varphi_h \\ &= \Delta_\alpha + \mathcal{F} \end{aligned} \tag{173}$$

where

$$\Delta_\alpha := \Delta - 2q^2 \alpha^\dagger \alpha \tag{174}$$

and

$$\begin{aligned} \mathcal{F} = &-2q^2(\alpha^\dagger h + \alpha h^\dagger) \\ &- 2q^2 \left\{ h^\dagger h - \alpha^\dagger \alpha \left(q^2 \Delta_\alpha^{-1}(\alpha h^\dagger - \alpha^\dagger h) \right) \left(q^2 \Delta_\alpha^{-1}(\alpha h^\dagger - \alpha^\dagger h) \right) \right. \\ &\left. + (\alpha^\dagger h - h^\dagger \alpha) q^2 \Delta_\alpha^{-1}(\alpha h^\dagger - \alpha^\dagger h) \right\}. \end{aligned} \tag{175}$$

The latter expresses $\mathcal{F}$ as an explicit sum of first and second order terms,

$$\mathcal{F} := \overset{(1)}{\mathcal{F}} + \overset{(2)}{\mathcal{F}} \tag{176}$$

[9] More precisely, actual normal coordinates would be the components of an expansion of the coordinate vector h in terms of an orthonormal basis for the tangent space, $T_\alpha \mathcal{S}$, to $\mathcal{S}$ at the point $\varphi = \alpha$. Since there is no apparent 'canonical' choice for such a basis we shall leave it unspecified in the discussion to follow. In terms of any such (herein suppressed) choice of actual normal coordinates, however, the metric at $\varphi = \alpha$ would simplfy to an explicitly 'Cartesian' form.

with

$$\overset{(1)}{\mathcal{F}} = -2q^2(\alpha^\dagger h + \alpha h^\dagger). \tag{177}$$

What we actually need however is the inverse operator $\Delta_{\varphi_h}^{-1}$ expanded to second order in h.

Note, however, that, for any field $\mathcal{B}$ lying in the range of $\Delta_{\varphi_h}^{-1}$, we have

$$\begin{aligned} \mathcal{B} &= \Delta_{\varphi_h}(\Delta_{\varphi_h}^{-1}\mathcal{B}) \\ &= (\Delta_\alpha + \mathcal{F})(\Delta_{\varphi_h}^{-1}\mathcal{B}) \end{aligned} \tag{178}$$

so that

$$\begin{aligned} \Delta_{\varphi_h}^{-1}\mathcal{B} &= \Delta_\alpha^{-1}\mathcal{B} - \Delta_\alpha^{-1}\left[\mathcal{F}(\Delta_{\varphi_h}^{-1}\mathcal{B})\right] \\ &= \Delta_\alpha^{-1}\mathcal{B} - \Delta_\alpha^{-1}\left[\mathcal{F}\left(\Delta_\alpha^{-1}\mathcal{B} - \Delta_\alpha^{-1}\left[\mathcal{F}(\Delta_{\varphi_h}^{-1}\mathcal{B})\right]\right)\right] \\ &= \Delta_\alpha^{-1}\left\{\mathcal{B} - \mathcal{F}\left(\Delta_\alpha^{-1}\left[\mathcal{B} - \mathcal{F}(\Delta_\alpha^{-1}\mathcal{B})\right]\right)\right\} \\ &\quad + \mathcal{O}(|h|^3) \end{aligned} \tag{179}$$

One could have iterated the intermediate steps above to get the result expressed to an arbitrary high order in h but, for the present purposes, the formula given here will suffice.

To evaluate the transformed kinetic energy we need to apply $\Delta_{\varphi_h}^{-1}$ to the specific quantity

$$\mathcal{B} = (\varphi_h^\dagger)_{,0}\varphi_h - (\varphi_h)_{,0}\varphi_h^\dagger. \tag{180}$$

Expanding this expression out through the use of (172) one arrives at

$$\mathcal{B} = \overset{(0)}{\mathcal{B}} + \overset{(1)}{\mathcal{B}} + \overset{(2)}{\mathcal{B}} \tag{181}$$

where

$$\overset{(0)}{\mathcal{B}} := (\alpha h_{,0}^\dagger - \alpha^\dagger h_{,0}) \tag{182}$$

$$\begin{aligned} \overset{(1)}{\mathcal{B}} = \Big[& hh_{,0}^\dagger - h^\dagger h_{,0} - (\alpha h_{,0}^\dagger + \alpha^\dagger h_{,0})q^2\Delta_\alpha^{-1}(\alpha h^\dagger - a^\dagger h) \\ & + (\alpha^\dagger h + h^\dagger \alpha)q^2\Delta_\alpha^{-1}(\alpha^\dagger h_{,0} - \alpha h_{,0}^\dagger)\Big] \end{aligned} \tag{183}$$

and

$$\begin{aligned}\overset{(2)}{\mathcal{B}} := \Big[&2(\alpha^\dagger h - h^\dagger \alpha) q^2 \Delta_\alpha^{-1} (\alpha h^\dagger - \alpha^\dagger h) \\ &- 2\alpha^\dagger \alpha \left(q^2 \Delta_\alpha^{-1} (\alpha h^\dagger - \alpha^\dagger h) \right) \left(q^2 \Delta_\alpha^{-1} (\alpha h^\dagger - \alpha^\dagger h) \right) \\ &+ 2h^\dagger h \Big] q^2 \Delta_\alpha^{-1} (\alpha^\dagger h_{,0} - \alpha h_{,0}^\dagger).\end{aligned} \tag{184}$$

A useful identity satisfied by the $\overset{(i)}{\mathcal{B}}$ and $\overset{(i)}{\mathcal{F}}$ is:

$$\overset{(2)}{\mathcal{B}} - \overset{(2)}{\mathcal{F}} \Delta_\alpha^{-1} \overset{(0)}{\mathcal{B}} = 0. \tag{185}$$

Assembling these various components for the kinetic energy $\mathcal{K}_\varphi$ and retaining terms explicitly only through second order in h one finally arrives at:

$$\begin{aligned}\mathcal{K}_\varphi = &\int_{\mathbb{R}^3} d^3x \left\{ h_{,0}^\dagger h_{,0} - \frac{q^2}{2} (\alpha h_{,0}^\dagger - \alpha^\dagger h_{,0}) \Delta_\alpha^{-1} (\alpha h_{,0}^\dagger - \alpha^\dagger h_{,0}) \right\} \\ &- \frac{q^2}{2} \int_{\mathbb{R}^3} d^3x \left\{ (\overset{(1)}{\mathcal{B}} - \overset{(1)}{\mathcal{F}} \Delta_\alpha^{-1} \overset{(0)}{\mathcal{B}}) \Delta_\alpha^{-1} (\overset{(1)}{\mathcal{B}} - \overset{(1)}{\mathcal{F}} \Delta_\alpha^{-1} \overset{(0)}{\mathcal{B}}) \right\} \\ &+ O(|h|^3)\end{aligned} \tag{186}$$

where

$$\begin{aligned}\overset{(1)}{\mathcal{B}} - \overset{(1)}{\mathcal{F}} \Delta_\alpha^{-1} \overset{(0)}{\mathcal{B}} = &2i\epsilon_{ab} \left[h_{,0}^a + \epsilon^{af} \alpha_f 2q^2 \Delta_\alpha^{-1} (\epsilon_{cd} h_{,0}^c \alpha^d) \right] \\ &\times \left[h^b + \epsilon^{bg} \alpha_g 2q^2 \Delta_\alpha^{-1} (\epsilon_{mn} h^m \alpha^n) \right]\end{aligned} \tag{187}$$

wherein

$$\alpha_f = \delta_{fg} \alpha^g = \alpha^f, \qquad \epsilon_{cd} = \delta_{cm} \delta_{dn} \epsilon^{mn} = \epsilon^{cd} \tag{188}$$

$$h = h^1 + ih^2, \qquad \alpha = \alpha^1 + i\alpha^2 \tag{189}$$

$$h^\dagger = h^1 - ih^2, \qquad \alpha^\dagger = \alpha^1 - i\alpha^2 \tag{190}$$

and $\epsilon^{ab} = -\epsilon^{ba}$ with $\epsilon^{12} = 1$ as before.

Noting that

$$\begin{aligned}\alpha h_{,0}^\dagger - \alpha^\dagger h_{,0} &= -2i\epsilon_{cd} \alpha^c h_{,0}^d \\ &= -\frac{2i}{c} \epsilon_{cd} \alpha^c h_{,t}^c\end{aligned} \tag{191}$$

and recalling Eq. (149) it is straightforward to verify that the first integral on the right hand side of Eq. (186) is simply 1/2 the squared norm of the velocity vectors $h_{,t}$ evaluated in the metric at $\varphi = \alpha$. As explained in the footnote for (171) this expression would simplify to purely 'Cartesian' form if $h_{,t}$ were expanded in actual normal coordinates there.

From the classical, Riemannian result for the expansion of a metric in normal coordinates it follows that the second integral on the right hand side of Eq. (186) is $-1/6$ of the curvature tensor of the metric (149) at $\varphi = \alpha$ evaluated, on both its first and last pair of 'slots', on the tangent plane spanned by the vectors h and $h_{,t}$. As such it corresponds (up to the usual normalization factor expressible in terms of the 'dot' products of these vectors) to the sectional curvature of this metric at the point α. Again, as explained in the previous footnote, this expression would directly yield the normal coordinate components of the sectional curvature at α if the vectors h and $h_{,t}$ were both expressed in a common orthonormal basis for the tangent space $T_\alpha \mathcal{S}$.

Furthermore, in view of the factors of i in the defining equation (187) of $\overset{(1)}{\mathcal{B}} - \overset{(1)}{\mathcal{F}} \Delta_\alpha^{-1} \overset{(0)}{\mathcal{B}}$ and of the negativity of the operator Δ_α defined by Eq. (115), it is clear that the curvature defined via Eq. (186) is everywhere non-negative (i.e., $\forall\ \alpha$ and for any pair $\{h, h_{,t}\}$ in $T_\alpha \mathcal{S}$) but also that it vanishes on those 2-planes in $T_\alpha \mathcal{S}$ for which $\overset{(1)}{\mathcal{B}} - \overset{(1)}{\mathcal{F}} \Delta_\alpha^{-1} \overset{(0)}{\mathcal{B}}$ vanishes.

The authors have not, so far, decided which regularization scheme fits most naturally with their overall *Euclidean-signature semi-classical* program. Such a decision is not needed until the higher order, quantum 'loop corrections' to field theoretic problems are under construction. These latter however (as one can see from sections IIB and IVB of Ref. [10] which treats the analogue quantum mechanical systems) will be governed entirely by the integration of first order, linear transport equations of a comparatively elementary type. By contrast we have instead focussed our efforts so far on solving the analytically more challenging, *uniquely nonlinear* functional partial differential equations for the fields of interest — namely the corresponding Euclidean-signature vanishing-energy functional Hamilton-Jacobi equations (cf., Sections 3.2 and 3.3 herein).

Until we do settle upon an appropriate regularization scheme we cannot, consistently, carry out the regularized construction of the relevant orbit space Ricci tensors for our program (or, for that matter, their loop corrected Bakry-Émery 'enhancements'). One hopes though, as is often the case in quantum field theory, that the result aimed for (e.g., positivity of the relevant Bakry-Émery Ricci tensor) will not crucially depend upon the method of regularization employed.

Acknowledgements

Moncrief is grateful to the Swedish Royal Institute of Technology (KTH) for hospitality and support during a visit in March 2015 and especially to Lars Andersson for pointing out the relevance of mathematical literature on Bakry-Émery Ricci tensors to the research discussed herein. The authors are also grateful to the Albert Einstein Institute in Golm, Germany, the Institut des Hautes Études Scientifiques in Bures-sur-Yvette, France, the Erwin Schrödinger Institute and the University of Vienna in Vienna, Austria for the hospitality and support extended to several of us during the course of this research.

References

[1] I. M. Singer. The geometry of the orbit space for non-Abelian gauge theories. *Phys. Scr.*, 24:817–820, 1981. MR0639408

[2] O. Babelon and C.M. Viallet. The Riemannian geometry of the configuration space of gauge theories. *Commun. Math. Phys.*, 81:515–525, 1981. MR0634446

[3] S. N. Vergeles. Some properties of orbit space in Yang-Mills theory. *Lett. Math. Phys.*, 7:399–406, 1983. MR0719853

[4] A. Lichnerowicz. *Géométrie des groupes de transformations.* Dunod, Paris, 1958. (23:A1329). MR0124009

[5] S. B. Myers. Riemannian manifolds with positive mean curvature. *Duke Math. J.*, 8:401–404, 1941. MR0004518

[6] Jun Ling. The first eigenvalue of a closed manifold with positive Ricci curvature. *Proc. Am. Math. Soc.*, 134:3071–3079, 2006. MR2231634

[7] D. Yang. Lower bound estimates of the first eigenvalue for compact manifolds with positive Ricci curvature. *Pac. J. Math.*, 190:383–398, 1999. MR1722898

[8] L. Andersson. The Bonnet-Myers theorem is true for Riemannian Hilbert manifolds. *Math. Scand.*, 58:236–238, 1986. MR0860881

[9] Note in particular that geodesic curves of infinite proper length of purely 'polarized' connections (i.e., ones for which the Lie brackets all vanish) exist along which the magnetic energy monotonically increases without bound.

[10] V. Moncrief, A. Marini, and R. Maitra. Modified semi-classical methods for nonlinear quantum oscillations problems. *J. Math. Phys.*, 53:103516–103567, 2012. MR3050612

[11] A. Marini, R. Maitra, and V. Moncrief. Euclidean signature semi-classical methods for bosonic field theories: interacting scalar fields. *Annals of Mathematical Sciences and Applications*, 1:3–55, 2016. MR3876483

[12] R. Maitra, A. Marini, and V. Moncrief. Euclidean signature semi-classical methods for bosonic field theories: Yang-Mills fields (title tentative). In preparation. See also, by the same authors, 'A Euclidean-Signature Semi-Classical Program', which is scheduled to appear in a special edition of *Communications in Analysis and Geometry* celebrating the 75th birthday of Karen Uhlenbeck. MR3876483

[13] J. Lott. Some geometric properties of the Bakry-Émery-Ricci tensor. *Comment. Math. Helv.*, 78:865–883, 2003. MR2016700

[14] G. Wei and W. Wylie. Comparison geometry for the Bakry-Émery Ricci tensor. *J. Differential Geom.*, 83:337–405, 2009. MR2577473

[15] R. G. Newton. *Scattering Theory of Waves and Particles*. Dover, 2013. See especially Section 7.3. MR1947260

[16] B.F. Hatfield. Gauge invariant regularization of Yang-Mills wave functionals. *Phys. Lett. B*, 154:296–302, 1985. MR0789044

[17] S. Krug. *The Yang-Mills Vacuum Wave Functional in 2+1 Dimensions*. PhD thesis, Department de Física, Universitat Autònoma de Barcelona, January 2014.

[18] M. Dimassi and J. Sjöstrand. *Spectral Asymptotics in the Semi-Classical Limit*. Cambridge University Press, 1999. See especially Chapters 1–3 and related references cited therein. MR1735654

[19] B. Helfer. *Semi-Classical Analysis for the Schrödinger Operator and Applications*. Springer-Verlag, Berlin Heidelberg, 1988. For more advanced topics, see [20]. MR0960278

[20] B. Helfer and J. Sjöstrand. Multiple wells in the semi-classical limit I. *Communications in Partial Differential Equations*, 9:337–408, 1984. MR0740094

[21] M. Brack and R. K. Bhaduri. *Semiclassical Physics (Frontiers in Physics)*. Westview Press, 2008. MR1976260

[22] A. M. Ozorio de Almeida. *Hamitonian Systems: Chaos and Quantization*. Cambridge Press, 1988. MR0985103

[23] A. D. Stone. Einstein's unknown insight and the problem of quantizing chaos. *Physics Today*, 58:37–43, 2005.

[24] These results were derived by Shilong (Peter) Tang during the course of completing a senior physics project at Yale University (unpublished, May 2016).

[25] V. P. Maslov and M. V. Fedoriuk. *Semi-Classical Approximation in Quantum Mechanics*. Reidel, 1981. MR0634377

[26] R. Abraham and J. Marsden. *Foundations of Mechanics*. Benjamin/Cummings, 1979. See Section 7.2. MR0515141

[27] R. Maitra. *Mathematically Rigorous Quantum Field Theories with a Nonlinear Normal Ordering of the Hamiltonian Operator*. PhD thesis, Department of Mathematics, Yale University, 2007. MR2711186

[28] J. A. Wheeler. *Geometrodynamics (Topics of Modern Physics, volume 1)*. Academic Press, London, 1962.

[29] R. Jackiw. Introduction to the Yang-Mills quantum theory. *Reviews of Modern Physics*, 52:661–673, 1980. MR0596015

[30] V. Khoze. The vacuum theta-angle is zero in non-Abelian gauge theories. *Physics Letters B*, 328:387–391, 1994.

[31] K. K. Uhlenbeck. Connections with L^p bounds on curvature. *Comm. Math. Phys.*, 83:31–42, 1982. MR0648356

[32] S. Sedlacek. A direct method for minimizing the Yang-Mills functional over 4-manifolds. *Comm. Math. Phys.*, 86:515–527, 1982. MR0679200

[33] A. Marini. Dirichlet and Neumann boundary value problems for Yang-Mills connections. *Comm. Pure Appl. Math.*, 45:1015–1050, 1992. MR1168118

Vincent Moncrief
Department of Physics and Department of Mathematics
Yale University
P.O. Box 208120
New Haven, CT 06520
USA
E-mail address: vincent.moncrief@yale.edu

Antonella Marini
Department of Mathematics
Yeshiva University
500 West 185th Street
New York, NY 10033
USA
Department of Mathematics
University of L'Aquila
Via Vetoio
67010 L'Aquila, AQ
Italy
E-mail address: marini@yu.edu

Rachel Maitra
Department of Applied Mathematics
Wentworth Institute of Technology
550 Huntington Avenue
Boston, MA 02115-5998
USA
E-mail address: maitrar@wit.edu

Received February 26, 2019