Calculation of eigenvalues of a strongly chaotic system using Gaussian wave-packet dynamics

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We apply the approximate dynamics derived from the Gaussian time-dependent variational principle (TDVP) to the Hamiltonian $\hat{H}=\frac{1}{2}(\hat{p}_x^2+\hat{p}_y^2)+\frac{1}{2}\hat{x}^2\hat{y}^2$, which is strongly chaotic in the classical limit. We are able to calculate, essentially analytically, low-lying eigenvalues for this system. These approximate eigenvalues agree within a few percent with the numerical results. We believe that this is the first example of the use of TDVP dynamics to compute individual eigenvalues in a nontrivial system and one of the few such computations in a chaotic system by *any* method. [S1063-651X(97)07407-2]

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I. INTRODUCTION

Gaussian approximations to quantum mechanics have been utilized successfully in many contexts including quantum field theory [1], the dynamics of hydrogen plasma [2], semiclassical propagation methods [3,4], quantum control [5], and the study of ''quantum chaos'' [6]. The primary motivation for their popularity is simplicity of computation: Gaussians are easily parameterized by the c number variables specifying the centroid (average variables) and spread (fluctuation variables) and their dynamics are essentially classical, apart from the computation of a phase which is a crucial element. Further, Gaussians arise naturally in the coherent state representation of quantum mechanics [7] and in the $N=\infty$ limit (where N is number of degrees of freedom) of many-body systems [8]. There are a variety of Gaussian approximations including: (1) a variational approximation usually derived through the time-dependent variational principle (TDVP) [1,9,10], (2) a recently introduced quadratic-order Gaussian approximation [4], (3) Heller's method [3], which is a non-self-consistent truncation of (2), and (4) the multiple classical trajectory version of Heller's method [11]. A further level of approximation yields the Gaussian effective potential method, which consists of an adiabatic elimination of the time dependence of the fluctuation variables in the TDVP dynamics [12].

The widespread use of these methods raises the question of their validity and range of applicability [13]. It has been argued that in the presence of chaos, semiclassical approximations to quantum mechanics should break down on a logarithmic time scale $t_c \sim 1/\lambda \log(1/\hbar)$, where λ is the largest Lyapunov exponent of the underlying classical mechanics, and $\hbar$ is Planck's constant. Computations with the multiple trajectory Gaussian approximation has demonstrated that this may be a pessimistic estimate [11]. Recently, the validity of the TDVP approximation has also been considered. Apart from the chaos in the underlying classical system, it has been shown that the approximate quantum dynamics derived from the TDVP may be chaotic even when the classical limit is not [14]. This has led to the argument [15] that the TDVP Gaussian approximation fails in the presence of chaos. However, it has been shown that this anomalous chaotic behavior persists even when exact numerical computations are made [16]. It is argued, in fact, that this chaos is a signature of the complicated nature of the spectrum involved in the exact quantum dynamics [4,17]. Further, recent work by Habib [18] shows that *all* Gaussian approximations to Schrödinger's equation are identical to the same approximation to the *classical* Liouville equation, although the classical versions do not have any phase information. This result clarifies that $\hbar$ is a kinematical constant in these approximations, providing a scale for the ''smoothing'' of the dynamics and reinterprets the ''quantum effects'' included in Gaussian approximations. It does not invalidate the results of the quantum Gaussian approximations, although it does require these results to be understood in kinematical rather than dynamical terms. The result also emphasizes that quantum dynamics are better approximated by classical Liouville dynamics rather than Hamilton's equations for point trajectories [19].

It is thus clear that Gaussian approximations should be used and interpreted with caution. However, as we shall demonstrate in this paper, the TDVP Gaussian approximation *does* yield accurate results even in the presence of chaos, in a system where other approximations fail. The TDVP dynamics can be used to compute eigenvalues [20,4] through an extension of the Einstein-Brillouin-Keller (EBK) quantization method [21]. We use this method to compute eigenvalues for the two-dimensional coupled quartic oscillator

$$\hat{H}=\frac{\hat{p}_x^2+\hat{p}_y^2}{2}+\frac{1}{2}\hat{x}^2\hat{y}^2. \tag{1}$$

This system is highly chaotic classically [22]; it was believed till recently to be ergodic, and the integrable regions of phase space occupy less than 0.005% of the volume. The quantal Hamiltonian also resists numerical analysis; large basis sets do not suffice for quantization [23]. It is usual for numerical ease to add a term such as $\beta(\hat{x}^4+\hat{y}^4)$ to the potential and to analyze the system in the limit $\beta \to 0$. The traditional meth-

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ods for semiclassical quantization fail for this particular system. Firstly, the EBK method cannot be applied because of the chaos in the system—there are no stable torii to use for quantization. The alternative methods developed in the field of quantum chaos [6] also do not work. The most prominent of these, the trace formula method, starts from Feynman's path-integral representation of quantum mechanics, and through a sequence of stationary phase approximations, derives the eigenvalues of the quantum system as poles in a weighted sum over the unstable periodic orbits of the classical system [24]. Recent successes in other systems [24,25] notwithstanding, the systematic enumeration of the unstable periodic orbits of the classical system has not been achieved for this particular system. Another alternative, Heller's approach [3], which computes an approximate time-dependent wave function $\langle\Psi(t)|$ and Fourier transforms the overlap $\langle\Psi(t)|\Psi(0)\rangle$, fails because of the inherent instability of the truncation, as argued in a previous qualitative [4] analysis in model potentials. In the same paper, we demonstrated that the TDVP dynamics restores stability to systems where the truncated Gaussian dynamics fail; in fact, the TDVP dynamics can be stable even when the *classical* dynamics are unstable. This is precisely what happens in the system given by Eq. (1): An infinite set of unstable periodic orbits is stabilized by the ''quantal fluctuation'' terms in the TDVP method. These orbits can then be used to compute approximate eigenvalues for a symmetry subspace of this system. Remarkably, these are obtained *analytically* (barring a numerical integral). Further, these results are obtained with $\beta=0$, i.e., the regime where even large basis-set calculations fail to converge. The high degree of chaos in the system and the fact that we use $\hbar=1$ in our calculations suggests the näive perspective that the classical-like TDVP approach is then far from its region of validity. However, our results are extremely accurate when compared with the ''exact'' numerical results over a substantial range for the lowest-lying eigenvalues. Thus, while there is no suggestion that this method can always be used in the presence of chaos to successfully approximate quantum dynamics, our results indicate that it can certainly be used with care in some circumstances.

In Sec. II, we shall briefly review the dynamical equations for the TDVP method, including the construction of a quantization rule. In the third section, we apply this method to Eq. (1), comparing the method in the process to the usual semiclassical methods. We then discuss the results and argue that the regime of validity of the method is the low quantum-number regime, contrary to the usual intuition derived from the correspondence principle that classical-like approximations work best in the high quantum-number regime [6]. We thus suggest that the TDVP Gaussian approximation works best as a technique complementary to the usual semiclassical methods.

II. TDVP GAUSSIAN DYNAMICS

The usual derivation of these dynamics proceeds from Dirac's time-dependent variational principle [9,10]; this posits an action of the form $\Gamma=\int dt\langle\Psi,t|i\hbar\partial/\partial t-\hat{H}|\Psi,t\rangle$. The general requirement that $\delta\Gamma=0$ yields the Schrödinger equation and its complex conjugate. The true solution is approximated by restricting $|\Psi(t)\rangle$ to a subspace of the full Hilbert space and setting $\delta\Gamma=0$ within this subspace. In particular, this restriction may be to the space of general Gaussians [1]. We have derived these same dynamics [14,4] in a somewhat more intuitive fashion from Ehrenfest's Theorem. We start with the equations for the centroid variables and make a Taylor expansion around the centroid with the higher moments of the wave function. These moments follow the usual Heisenberg dynamics, yielding in general an infinite system of equations. We render this system finite by projecting onto the space of Gaussians; this system of equations are identical to those derived from the TDVP.

We have been able to represent these dynamics as an extended *classical gradient system* for the average and fluctuation variables with dynamical equations

$$\frac{dx}{dt}=p, \tag{2}$$

$$\frac{dp}{dt}=-\sum_{m=0}^{m=\infty}\frac{\rho^{2m}}{m!2^m}V^{(2m+1)}(x), \tag{3}$$

$$\frac{d\rho}{dt}=\Pi, \tag{4}$$

$$\frac{d\Pi}{dt}=\frac{\hbar^2}{4\rho^3}-\sum_{m=1}^{m=\infty}\frac{\rho^{2m-1}}{(m-1)!2^{m-1}}V^{(2m)}(x), \tag{5}$$

and a Hamiltonian

$$H_{\rm ext}=\frac{p^2}{2}+\frac{\Pi^2}{2}+V_{\rm ext}(x,\rho); \tag{6}$$

$$V_{\rm ext}(x,\rho)=V(x)+\frac{\hbar^2}{8\rho^2}+\sum_{m=1}\frac{\rho^{2m}}{m!2^m}V^{(2m)}(x), \tag{7}$$

where the subscript ext indicates the ''extended'' potential and Hamiltonian and $V^{(n)}=\partial^n V/\partial x^n|_{\langle\hat{x}\rangle}$. The coordinate variables for the extended Hamiltonians are x,ρ, and their canonically conjugate momenta are p,Π and are related to the moments of the Gaussian $\Psi(x,p,\rho,\Pi,t)$ as follows:

$$\langle\hat{x}\rangle\equiv x, \tag{8}$$

$$\langle\hat{p}\rangle\equiv p, \tag{9}$$

$$\langle\Delta x\Delta p+\Delta p\Delta x\rangle\equiv 2\rho\Pi, \tag{10}$$

$$\langle\Delta x^{2m}\rangle=\frac{(2m)!\rho^{2m}}{m!2^m}, \tag{11}$$

$$\langle\Delta x^{2m+1}\rangle=0, \tag{12}$$

$$\rho^2\langle\Delta p^2\rangle=\frac{\hbar^2}{4}+\rho^2\Pi^2. \tag{13}$$

The first three relationships Eqs. (8–10) are *definitions* and Eqs. (11) and (12) are a consequence of the Gaussian ansatz. Equation (13) is a kinematical constraint arising entirely

from choosing the equality in the uncertainty principle relationship; it is the only way in which $\hbar$ enters this approximation.

In this method, the fluctuation and average variables are treated on the same footing and the phase space is dimensionally consistent: ρ has the dimensions of length and Π that of momentum. The geometry of the space is thus identical to that of an ordinary classical system—it is a Cartesian space, a manifold $\mathcal{R}(2N)$ defining the extended phase space. There is also an equation for the phase of the wave function: If we define λ as $|\Phi,t\rangle \equiv \exp[i\lambda(t)/\hbar]|\Psi,t\rangle$ it is simple to derive from Schrödinger's equation the equations for $\lambda=\lambda_D+\lambda_G$, with the first part

$$\lambda_D=-\int_0^t d\tau\langle\hat{H}\rangle=-tH_{\text{ext}} \tag{14}$$

corresponding to the dynamical phase. The second part is the geometrical phase

$$\lambda_G=\int_0^t d\tau\left\langle i\hbar\frac{\partial}{\partial\tau}\right\rangle=\int_0^t d\tau\left(\frac{\dot{\rho}\Pi-\dot{\Pi}\rho}{2}+p\dot{x}\right). \tag{15}$$

For cyclic evolution this is the Aharanov-Anandan form of ''Berry's phase'' [26]; it depends only on the geometry of the evolutionary path in phase space and can be written as

$$\lambda_G(C)=\oint_C \mathbf{P}\cdot\mathbf{dQ}, \tag{16}$$

where $\mathbf{P}\equiv(p,\Pi)$ and $\mathbf{Q}\equiv(x,\rho)$. The equation for the phase, along with the Hamiltonian equations of motion for the evolution of the wave function parameters constitute the TDVP dynamics. This lies on a space $\mathcal{R}(2N)\times S(1)$; for the case just considered $N=2$, the result is completely general, however.

We now provide a constructive argument [4] for obtaining eigenfunctions and eigenvalues, which is equivalent to imposing a single-valuedness constraint on stationary wave functions [20] in the extended phase space. Note that an eigenfunction for the extended dynamics is one whose parameters are *invariant* under the evolution. We see readily that a periodic orbit (PO) solution to Hamilton's equations Eqs. (2)–(5) is invariant on the $\mathcal{R}(2N)$ subspace; however, each point along the PO acquires a phase factor during the evolution. The dynamical phase is the same for all the points along the PO and can be factored as a global phase. The geometrical part λ_G for the PO is crucial: We note that a PO$\times\lambda_G$, such that the periodic evolution of λ_G on $\mathcal{S}(1)$ is *commensurate* with that of the PO on $\mathcal{R}(2N)$ is a function invariant on entire space $\mathcal{R}(2N)\times\mathcal{S}(1)$ and is hence an *eigenfunction*. The commensurability of the phase translates to the relation

$$\lambda_G(PO)=\frac{1}{2\pi}\oint_{PO}\mathbf{P}\cdot\mathbf{dQ}=n\hbar, \tag{17}$$

where we have used Eq. (16). Thus, the eigenfunction is a weighted sum (the weight factor at each point being the appropriate geometrical phase) over the points of the commensurate periodic orbit and the eigenvalue is H_{ext} for that PO. This rule is the same as the ''old'' quantization rule of Bohr and Sommerfeld; however, it applies in the *extended* phase space, as opposed to the classical phase space and thus does not have the same meaning. In particular, there are no Maslov-Morse corrections [21] to this rule, since there are no singularities in the Gaussian representation. It can be shown [27,4] that the ''spread'' variables ρ,Π explicitly take care of these corrections. In general, this quantization condition will give results different from the EBK rule (the POs are in the extended space) but always incorporates the Maslov correction. The extension of this argument from POs to invariant torii goes through easily [20] and leads to a general quantization rule

$$\frac{1}{2\pi}\oint_{C_i}\mathbf{P}\cdot\mathbf{dQ}=n_i\hbar, \tag{18}$$

where the closed integral is now taken over the ith irreducible contour around the torus and the quantum numbers n_i are labeled accordingly. This is exactly Einstein's generalization [28] of the Bohr-Sommerfeld rule to invariant torii.

The system of equations derived by Heller [3] for the semiclassical evolution of Gaussian wave packets obtain as truncations of Eqs. (2) and (3) to $\mathcal{O}(\rho^0)$ and of Eqs. (4) and (5) to $\mathcal{O}(\rho^1)$. This arguably [4] inconsistent semiclassical system of equations destroys the Hamiltonian structure of the dynamics, leading to nonunitary evolution [29]. A consistent truncation to $\mathcal{O}(\rho^1)$) for this system retains the Hamiltonian structure of the TDVP method and has been termed extended semiclassical dynamics [4]: All the advantages of the TDVP method applies to the extended semiclassical method, including the definition of a Poisson bracket, and the existence of a unitary propagator and an analytic quantization method. Unlike the TDVP method, Heller's Gaussian dynamics and the extended semiclassical dynamics arise as ''controlled'' first-order expansions; their validity can thus be formally evaluated [13] and these are hence attractive approximations. However, the truncation of the dynamical equations at the term involving the third derivative of the potential induces an unphysical instability, where the fluctuation variables grow without bound [4] even for simple one-dimensional anharmonic potentials like $V(x)=x^4$. In the TDVP dynamics, all orders of derivatives are maintained with a resummation of the moment expansion under a Gaussian ansatz; this yields behavior that is qualitatively similar to the exact long-term quantal behavior, in particular reproducing the appropriate stability. Thus, the TDVP method can stabilize unstable periodic orbits, which may then be used as above to obtain eigenvalues and eigenfunctions, as we now demonstrate.

III. EIGENVALUES FOR A CHAOTIC HAMILTONIAN

We now turn to the computation of eigenvalues for the Hamiltonian

$$\hat{H}=\frac{\hat{p}_x^2+\hat{p}_y^2}{2}+\frac{1}{2}\hat{x}^2\hat{y}^2+\beta(\hat{x}^4+\hat{y}^4). \tag{19}$$

Extensive numerical work [23,22] shows that the classical limit ($\hat{O}\to O$ for all operators) is a very strongly chaotic system, with few stable periodic orbits in the limit $\beta\to 0$. It

is easy to verify, however, the existence of an infinity of unstable periodic orbits along the diagonals of the potential. We also note here that the Hamiltonian displays a simple scaling relationship in energy [23]: A trajectory $(\mathbf{x}_1(t),\mathbf{p}_1(t))$ at an energy E_1 is related to a trajectory $(\mathbf{x}_2(t),\mathbf{p}_2(t))$ at an energy E_2 by

$$\mathbf{x}_2(\tau)=\left(\frac{E_2}{E_1}\right)^{1/4}\mathbf{x}_1(t), \tag{20}$$

$$\mathbf{p}_2(\tau)=\left(\frac{E_2}{E_1}\right)^{1/2}\mathbf{p}_1(t), \tag{21}$$

where τ is the rescaled time $\tau=(E_2/E_1)^{-1/4}$. This means that there is the same degree of strong chaos at all finite energies: There is no ''transition to chaos.'' Eckhardt, Hose, and Pollak have done a careful numerical analysis of the quantum system to show the presence of ''scars'' in the eigenfunctions [23]. They state that harmonic oscillator basis-set quantization with matrices of dimension 3240 do not provide converging eigenvalues for $\beta=0$; they have hence used $\beta=0.01$ for their analysis. The eigenfunctions of this Hamiltonian belong to the symmetry classes of the C_{4v} symmetry group which has eight elements (four reflections in the axes and diagonals and four rotations by $\pi/2$). The irreducible representations of this group split into four one-dimensional representations and one two-dimensional representation. They have restricted themselves to the four one-dimensional representations corresponding to wave functions which are (A) symmetric under $x\rightarrow y$, $x\rightarrow -x$, (B) antisymmetric, symmetric, (C) symmetric, antisymmetric, and (D) antisymmetric, antisymmetric, respectively, and have numerically obtained low-lying eigenvalues and eigenstates for this system.

We have applied the Gaussian wave-packet methods detailed above to this system with $\beta=0$. Of the three methods, the truncated Gaussian methods (both Heller's dynamics and the extended semiclassical system) fail, yielding unstable motion where the wave-packets spread without bound, irrespective of the value of β. This is easily established by noting that there exist one-dimensional projections in which this two-dimensional potential reduces to the anharmonic quartic potential considered above and the existence of a single unstable direction for the dynamics corresponds to instability in the global motion. This exposes one particular frailty of the truncated Gaussian approximations: they work well in systems that are close to harmonic only in the *particular* sense of being potentials of the form $V(x)=x^2+f(x)$ with the function $f(x)$ containing higher polynomials.

On the other hand, the TDVP method works excellently for this system; firstly, the dynamics are completely bounded. It is an interesting feature of this approach that even though there exist classically unbounded orbits along $x=0$ or $y=0$ (which are precisely what make the numerical quantal analysis through basis sets so difficult) the inclusion of the resummed moment terms via the variational approach restores stability to the problem. This effect has been termed ''quantum resuscitation'' in the context of the Gaussian effective potential [12]. The extended Hamiltonian for the TDVP [using $\Psi=\Phi(x)\Phi(y)$ and $\hbar=1$] is

$$H_{\rm ext}=\tfrac{1}{2}(p_x^2+p_y^2+\Pi_x^2+\Pi_y^2)+\frac{1}{8\rho_x^2}+\frac{1}{8\rho_y^2}+\frac{1}{2}(x^2+\rho_x^2)\times(y^2+\rho_y^2). \tag{22}$$

Note that the use of the factored wave functions explicitly restricts us to the one-dimensional representations. The dynamics of this extended Hamiltonian are, in general, chaotic. However, if we consider the subspaces of the one-dimensional representation noted above, we find that the first and third subspace can be studied by the symmetry-reduced version of $H_{\rm ext}$

$$H=\tfrac{1}{2}(p^2+\Pi^2)+\frac{1}{8\rho^2}+\frac{1}{4}(z^2+\rho^2)^2, \tag{23}$$

where (z,p) and (ρ,Π) are the canonically conjugate pairs.

We now demonstrate that this symmetry-reduced version of the *extended* Hamiltonian is explicitly integrable. To do so, we make the change of variables to spherical coordinates R,θ defined in the plane by: $z=R\cos\theta$; $\rho=R\sin\theta$. This transforms the Hamiltonian to

$$H=\frac{p_R^2}{2}+\frac{R^4}{4}+\frac{1}{R^2}\left[\frac{p_\theta^2}{2}+\frac{1}{8\sin^2\theta}\right]. \tag{24}$$

Since the factor multiplying $1/R^2$ is solely a function of θ, this is now in the right form to use Hamilton-Jacobi theory [30]. Through the separability just noted, therefore, we introduce Hamilton's characteristic functions W_R and W_θ and get the Hamiltonian-Jacobi equations

$$\frac{1}{2}\left(\frac{\partial W_\theta}{\partial\theta}\right)^2+\frac{1}{8\sin^2\theta}=k, \tag{25}$$

$$\frac{1}{2}\left(\frac{\partial W_R}{\partial R}\right)^2+\frac{R^4}{4}+\frac{k}{R^2}=E, \tag{26}$$

where E (the energy) and k are the constants of separation. We form action variables as usual

$$J_\theta=\frac{1}{2\pi}\oint d\theta\frac{\partial W_\theta}{\partial\theta} \tag{27}$$

$$=\frac{1}{2\pi}\oint d\theta\left(2k-\frac{1}{4\sin^2\theta}\right)^{1/2}, \tag{28}$$

$$J_R=\frac{1}{2\pi}\oint dR\frac{\partial W_R}{\partial R} \tag{29}$$

$$=\frac{1}{2\pi}\oint dR\left(2E-\frac{2k}{R^2}-\frac{R^4}{2}\right)^{1/2}. \tag{30}$$

The θ integral yields [31]

$$J_\theta=\frac{\alpha-1}{2}, \tag{31}$$

where α is introduced for convenience through $k\equiv\alpha^2/8$. The R integral is a complicated elliptic integral that can be evalu-

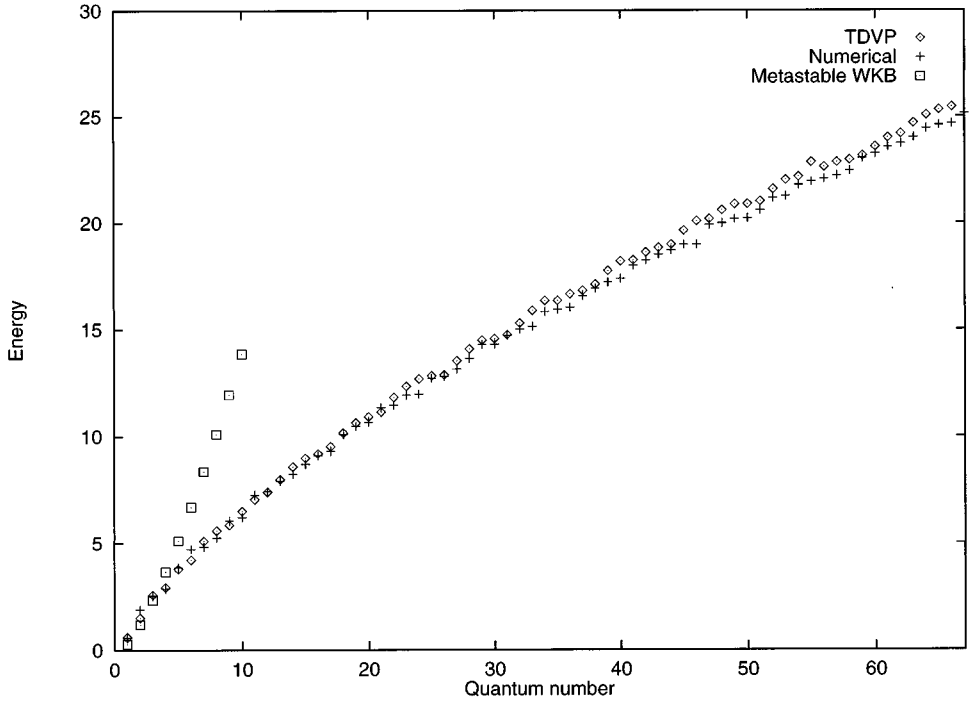

FIG. 1. Comparison of lowest eigenvalues in dimensionless units. Note that $\hbar=1$.

ated; however, it cannot be analytically inverted to yield the quantization condition. We, hence, leave it in quadrature

$$J_R=\frac{1}{2\pi}\oint dR\left(2E-\frac{(2J_\theta+1)^2}{4R^2}-\frac{R^4}{2}\right)^{1/2}. \qquad (32)$$

The existence of this integral demonstrates the integrability of the chosen symmetry subspace of the extended Hamiltonian. Since we now have a set of stable invariant torii in the extended space, we can proceed with the quantization as detailed above in a straightforward fashion. To wit: Eigenvalues correspond to torii with quantized actions in both variables R and θ. We follow this prescription by setting J_θ equal to a half-integer in the above equation [the symmetry-reduced form of the Hamiltonian only accumulates half the phase of the actual Hamiltonian which is why we use half-integers]; this yields a one-degree of freedom dynamical system in R which has only closed orbits. We then proceed as follows: We take various initial conditions and numerically integrate their dynamics over the closed orbit to compute the action $\oint P_R dR$. The orbits for which the action equals a half-integer then correspond to eigenfunctions and their conserved energy the associated eigenvalue. We show the results for the first 67 eigenvalues in Fig. 1, compared with the numerical results [32] of Eckhardt, Hose, and Pollak. We now note that the eigenvalues we have calculated essentially analytically agree within a few percent with the numerical results [23] over the substantial range of our calculations.

We emphasize that there is no possibility that the validity of the results can be attributed to the minute regions of stability of the classical phase space [33]. A moment's consideration shows that the use of the factored wave functions and the restriction $y(t)=x(t)\equiv z(t)$ for the symmetric dynamics corresponds to restricting our attention to the diagonals of the potential. That is, the dynamics of the Gaussian are restricted such that the centroid always travels always along the unstable periodic orbits along these diagonals. The few classical stable periodic orbits that do exist in this system lie far from this region and our results cannot be understood as affected by the presence of these orbits; the wave packet is not influenced by them.

Further, we note that there is a superficial similarity of these results to other work [34] that demonstrates the efficacy of Gaussian approximations in computing low-lying spectral features. However, those results depend on perturbations of a classically integrable Hamiltonians. As such, they were able to use standard quantal perturbation theory. This is not possible for Eq. (1). Further, since the classical dynamics is *ab initio* strongly chaotic, even the Gustavson-Birkoff quantization technique [35], which is an adaptation of classical perturbation theory, cannot be applied. In either case, there is nothing to perturb around for this system. This also emphasizes the nonperturbative aspect of the variational approximation.

It is clear that the TDVP method in this system takes advantage of the interesting feature of being able to use the infinity of periodic orbits along the diagonals of the potential. These orbits are classically *unstable*, and the formal application of the WKB quantization method to this unstable periodic orbit yields metastable states [36], where the eigenvalues have a real part (corresponding to the energy) and an imaginary part (corresponding to the lifetime of the state). Apart from the unphysical metastability of these states, the approximate energies thus obtained are valid only for the first few states—we show the limited accuracy in Fig. 1, where we have plotted the real parts of the first ten eigenvalues from this method. This same instability of the periodic orbit causes the breakdown of the truncated Gaussian semiclassical methods as well. However, the TDVP Gaussian an-

satz makes dynamics along these periodic orbits *stable*—an example of ''quantum resuscitation''—and our generalized quantization method succeeds.

There are more general considerations also: Note that, despite the high degree of chaos in the system, the potential is relatively benign for Gaussian approximations: It has only one minimum and no maxima. However, since it is a quartic well, this does not benefit the truncated approximations and we must turn to the fully resummed TDVP approximation to take advantage of this structure. Second, the high value of $\hbar$ is an advantage in this context. As recent work [37] demonstrates, at higher values of $\hbar$ the details of the classical phase-space structure are smoothed out in the quantal dynamics [see Fig. 2(a) of [37]], as reflected by the quantal eigenfunctions. Since $\hbar$ also sets the kinematical scale of smoothness for the TDVP Gaussian method [18], this means that both the exact quantal dynamics and our approximate version are effectively occurring in a smoother potential well than the classical point dynamics. Both these factors imply that distorted Gaussians can be expected to evolve without excessive error under such circumstances. Further, the smoothness permits the weighted superposition of Gaussians inherent in the TDVP eigenfunction ansatz to yield accurate results: The detailed structure of the wave functions may be argued to contribute rapidly oscillating terms that affect the computation of *averages* of observables in these states in a small way. Thus, eigenvalues, which are the average of the Hamiltonian operator, may be quite accurate even when the detailed dynamics of the variational approximation are not so. This also clarifies that the method is expected to be valid in the regime of the lowest-lying eigenvalues, contrary to the usual correspondence principle regime where classical-like approximations work best in the high quantum number regime [6]. This is supported by our results: they deviate slowly away from the numerical results as the quantum number increases.

Our results thus show that the degree of chaos in a classical problem does *not* necessarily limit the validity of the TDVP Gaussian dynamics. In a general case, chaos in the classical dynamics of a system coexists with complicated potential energy surfaces; Gaussian methods would hence apply only over a small range of parameters. However, there are systems that may be extremely chaotic, but possess the appropriate structure that enables the TDVP Gaussian approximation to work over a much larger range, especially in the high $\hbar$ regime; this explains the many successful applications [2], for instance. It is clear that these arguments need to be explored carefully in more situations.

In summary, we have analytically (barring a numerical integral) computed the lowest-lying eigenvalues of a classically strongly chaotic system. We believe that this is the first example of the use of TDVP dynamics to compute individual eigenvalues in a nontrivial system and one of the few such computations in a chaotic system by *any* method. These results compare extremely favorably with numerical results and show that the limits of validity of the TDVP method are not necessarily set by the degree of chaos in the classical system. Accurate quantum dynamical simulations are quite difficult and there is a great need for valid approximations [38]. Heller's truncated Gaussian approximation has already been shown [3] to be extremely useful for systems that can be explicitly written as perturbations around a harmonic minimum. It is intuitive that Gaussian approximations should continue have validity in potential wells, even in the presence of chaos; however, the truncated Gaussian methods fail in anharmonic systems. We believe that the TDVP Gaussian method is an excellent candidate for approximate quantum dynamics in these and other situations.

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