Semiclassical Quantization of Nonseparable Systems without Periodic Orbits

Franz Josef Weiper, Joachim Ankerhold, and Hermann Grabert
Fakultät für Physik, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Strasse 3, D-79104 Freiburg, Germany

Eli Pollak
Chemical Physics Department, Weizmann Institute of Science, 76100 Rehovot, Israel

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We present a new method for the semiclassical quantization of classically integrable as well as nonintegrable systems. The method is based on the semiclassical approximation of the equilibrium density matrix, using classical trajectories on the upside down potential surface. Periodic orbits do not play any special role. Explicit results are given for the case of the classically chaotic potential $kx^2y^2/2$. [S0031-9007(96)01277-X]

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Enormous progress has been made in the last two decades in understanding the semiclassical approximation to quantum mechanics. The semiclassical spectrum of bound states may be obtained using the Einstein-Brillouin-Keller method (EBK) for classically integrable systems [1]. If the system is not integrable, one resorts to the periodic orbit summation formula of Gutzwiller [2]. In both cases, the semiclassical density of states is obtained by finding either the periodic or the quasiperiodic orbits of the system. Both methods do not provide a semiclassical approximation for the wave function; other methods, such as the use of Gaussian wave packets in conjunction with the classical orbits, must be employed.

In this Letter we propose to use a semiclassical method, which is equally applicable to classically integrable and nonintegrable systems and which gives at the same time a good approximation to the quantum wave function. The central idea is the systematic use of the semiclassical approximation to the matrix elements of the imaginary time propagator

$$\rho(\mathbf{x},\mathbf{x}';\beta) \equiv \langle \mathbf{x}|e^{-\beta H}|\mathbf{x}'\rangle\,,$$

where $\mathbf{x}$ denotes a point in the n-dimensional configuration space, H is the Hamiltonian, and $\beta = 1/k_BT$ is the imaginary time in units of $\hbar$.

Consider, for example, the diagonal matrix element. It can be decomposed in terms of the exact eigenfunctions $\psi_i(\mathbf{x})$ and eigenvalues E_i of the Hamiltonian as

$$\rho(\mathbf{x},\mathbf{x};\beta) = \sum_{i=0}^{\infty} e^{-\beta E_i}|\psi_i(\mathbf{x})|^2. \tag{1}$$

If the imaginary time β is large enough (a more precise definition is given below) then only the ground state will contribute to the sum. The density $|\psi_0(\mathbf{x})|^2$ is independent of β and normalized, so that knowledge of the diagonal matrix element and its integral over $\mathbf{x}$ for times β that are sufficiently large will suffice to determine both the eigenvalue E_0 as well as the density $|\psi_0(\mathbf{x})|^2$. Having determined the ground state energy and density, one may subtract them off the sum given in (1) and repeat the process to get the first excited state energy and density. In this manner, one may peel off, state by state, the eigenvalues and densities. All that is needed is a "good" semiclassical estimate of the imaginary time propagator.

The semiclassical theory for the imaginary time propagator is rather old. Over sixty years ago, Wigner [3] found the leading order term in an $\hbar$ expansion of the partition function $\mathrm{tr}(e^{-\beta H})$. Feynman suggested the use of variational methods [4], based on the Bogoliubov inequality and a semiclassical expansion of the path integral. This approach was developed extensively by Kleinert [5,6]. The use of classical trajectories in imaginary time as a practical way for computing densities originates with Miller and coworkers [7]. However, none of these approaches was ever used in a systematic way to elucidate the quantum eigenvalues and densities of multidimensional systems.

Consider a system with two degrees of freedom for which the real time classical motion is chaotic. The Gutzwiller summation [2] may be used in principle, however, it is difficult to implement in practice because of the typically large numbers of periodic orbits that contribute to the sum, each with a different phase. While practical resummation schemes have been implemented, in the real time approach [8], one must still deal with a summation of terms with varying phases. In contrast, in imaginary time, the trajectories sum up with real negative exponents. Convergence of the sum over imaginary time trajectories may thus be expected to be fast.

Very recently, Weiper *et al.* [9] have demonstrated for a one-dimensional system that the semiclassical approximation to the propagator leads to reliable estimates of bound states and resonance energies as well as the associated densities. In the present paper, we demonstrate the applicability of the imaginary time semiclassical theory to a model system with two degrees of freedom whose real time dynamics is known to be largely chaotic.

The coordinate representation of the imaginary time propagator (the density matrix) of a quantum particle of mass m moving in the potential $V(\mathbf{x})$ may be written as an imaginary time path integral:

$$\rho(\mathbf{x},\mathbf{x}';\beta) = \int \mathcal{D}[\mathbf{x}] e^{-S[\mathbf{x}]/\hbar}. \tag{2}$$

The functional integral is over all paths $\mathbf{x}(\tau), 0 \le \tau \le \hbar\beta$ such that $\mathbf{x}(0) = \mathbf{x}$ and $\mathbf{x}(\hbar\beta) = \mathbf{x}'$. Each path is weighted by its Euclidean action

$$S[\mathbf{x}] = \int_0^{\hbar\beta} d\tau \left[\frac{m}{2}\dot{\mathbf{x}}^2 + V(\mathbf{x}) \right].$$

An arbitrary path in configuration space, parametrized by the time τ, may be written as $\mathbf{x}(\tau) = \mathbf{x}_{\rm cl}(\tau) + \mathbf{y}(\tau)$, where the classical path $\mathbf{x}_{\rm cl}(\tau)$ is the *imaginary time* solution of the classical equations of motion in the potential $V(\mathbf{x})$ [7], and $\mathbf{y}(\tau)$ describes fluctuations with the boundary conditions $\mathbf{y}(0) = \mathbf{y}(\hbar\beta) = 0$. The action may be decomposed into a classical action $S[\mathbf{x}_{\rm cl}]$ and a fluctuating part which comes from the fluctuation path $\mathbf{y}(\tau)$. The semiclassical estimate of the density is obtained by expanding the action appearing in the path integral (2) up to second order in the fluctuations about the classical path. The classical path minimizes the action and is the dominant contribution to the sum. If there exists a set $\{\mathbf{x}_{\rm cl}^{\alpha}\}$ of classical trajectories leading from the initial to the final point in the time interval $\hbar\beta$, one must sum the contributions from all of them. The semiclassical density matrix $\rho_{\rm sc}(\mathbf{x},\mathbf{x}';\beta)$ has the form

$$\rho_{\rm sc}(\mathbf{x},\mathbf{x}';\beta) = \sum_{\alpha} \frac{1}{\sqrt{J_\alpha}}\, e^{-S[\mathbf{x}_{\rm cl}^{\alpha}]/\hbar}, \tag{3}$$

where $J_\alpha = \det\{\delta^2 S[\mathbf{x}]/\delta\mathbf{x}(\tau_1)\delta\mathbf{x}(\tau_2)|_{\mathbf{x}=\mathbf{x}_{\rm cl}^{\alpha}}\}$ is the determinant describing the Gaussian integral over the quantum fluctuations. The details of evaluation of the determinant may be found in Refs. [4,6,10].

In this Letter we consider a quartic oscillator potential in two degrees of freedom [11], which has the form

$$V(\mathbf{x}) = \frac{k}{2}x^2y^2, \quad k > 0. \tag{4}$$

This potential does not have any stable fixed points. The classical trajectories are mostly chaotic, stable orbits do exist but are long, and the area of the stable phase space surrounding them is negligible [11]. It is this lack of integrable motion which makes the quartic potential a formidable challenge to semiclassical theory. It is useful to rewrite the problem in terms of the dimensionless variables: $X = (k\hbar^2\beta^2/m)^{1/2}x$, $Y = (k\hbar^2\beta^2/m)^{1/2}y$, $dt = d\tau/\hbar\beta$, and $\tilde{S} = S/\hbar$. Furthermore, all dimensionless classical trajectories scale according to $\mathbf{X}_{\rm cl}(t,1) = \alpha\mathbf{X}_{\rm cl}(\alpha t,\alpha)$, $\alpha > 0$, where $\mathbf{X}_{\rm cl}(t,\theta)$ is a path with $t \in [0,\theta]$. It therefore suffices to solve the classical equations of motion at a certain temperature to obtain the solutions at all temperatures.

The Hamiltonian with the quartic oscillator potential (4) has C_{4v} symmetry. This group has four nondegenerate irreducible representations labeled by A_1, A_2, B_1, and B_2. In addition, there is a doubly degenerate irreducible representation E. Hence the full density matrix can be written as

$$\rho(\mathbf{x},\mathbf{x}';\beta) = \sum_{g} \rho_g(\mathbf{x},\mathbf{x}';\beta), \tag{5}$$

where $g \in \{A_1, A_2, B_1, B_2, E\}$. To obtain the density matrix ρ_g for each representation separately one must properly symmetrize the full density matrix by taking into account off-diagonal matrix elements which are related to each other by the eight symmetry operations of the group. For example, the diagonal part of the density matrix associated with representation A_1 takes the form

$$\begin{aligned}\rho_{A_1}[\mathbf{x},\mathbf{x};\beta] =& [\varrho(x,y) + \varrho(-x,y) + \varrho(y,x) \\ &+ \varrho(-y,x) + \varrho(-y,-x) + \varrho(-x,-y) \\ &+ \varrho(x,-y) + \varrho(y,-x)]/8,\end{aligned}$$

where we put $\mathbf{x} = (x,y)$ and $\varrho(\pm x, \pm y)$ represents the matrix elements $\rho[(x,y),(\pm x,\pm y);\beta]$ of the full density matrix.

One of the interesting features of the imaginary time semiclassical approximation is that the contributing trajectories are proper solutions of a boundary value problem with fixed end points. In addition, apart from the low temperature region, the semiclassical density matrix ρ_g for a specific representation is determined only by at most eight trajectories [see Fig. 1(a)]. Note that for very low temperatures and for coordinates near the diagonal one can have more than one trajectory contributing to the full density matrix [cf. Fig. 1(b)]. The central idea of any semiclassical approximation is that the fluctuations about the classical paths are small. For the present potential, this assumption does not hold for very low temperatures. In particular, the accumulation of orbits along the diagonals ($x = \pm y$) implies bifurcations and associated large fluctuations. One may correct for these large fluctuations by going to higher order in the expansion about the classical orbit, as shown for one-dimensional systems in Ref. [12]. Extension of these methods to the quartic potential (4) will be considered elsewhere.

Having determined the density matrix, the free energy of the system is obtained from $F(\beta) = -\ln[Z(\beta)]/\beta$,

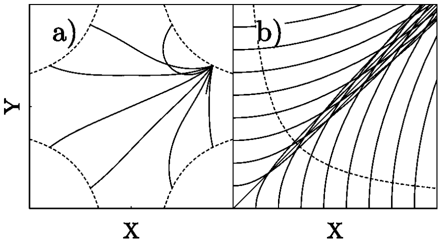

FIG. 1. Classical trajectories in the inverted potential (4). (a) Typical trajectories contributing to the matrix elements $\rho[\mathbf{x},(\pm x,\pm y);\beta]$ and $\rho[\mathbf{x},(\pm y,\pm x);\beta]$. (b) Low temperature trajectories in the first quadrant of configuration space. Dashed lines represent equipotential lines.

where

$$Z(\beta) = \int d\mathbf{x}\, \rho(\mathbf{x}, \mathbf{x}; \beta) = \sum_{i=0}^{\infty} e^{-\beta E_i} \tag{6}$$

is the partition function. As mentioned above, the density matrix (1) and also the partition function (6) can now be used to quantize a system within a semiclassical approximation. At a sufficiently large $\beta = \beta_0$ we first get $F(\beta_0) = E_0$ and then from the density matrix $|\psi_0(\mathbf{x})|^2$. Subtracting this ground state contribution from the full density matrix gives with the same procedure as before at a sufficiently large temperature $\beta_1 < \beta_0$ the energy E_1 and the density $|\psi_1(\mathbf{x})|^2$ of the first excited state, and so on state by state. Large β_i means that $\exp[-\beta_i(E_{i+1} - E_i)]$, $i = 0, 1, 2, \ldots$, is small compared to 1. This condition must be confirmed self-consistently. In principle, one should consider the limit $\beta \longrightarrow \infty$ to minimize the thermal error from contributions from excited states. On the other hand, the scaling properties of the scale invariant potential (4) imply that the semiclassical expansion parameter $\hbar$ corresponds to β^3. Thus the simple semiclassical approximation (3) becomes exact at high temperatures $\beta \longrightarrow 0$ but breaks down for very large β. As a consequence, semiclassical quantization of the system can be implemented by looking for an optimal intermediate value of β for which the thermal error is exponentially suppressed but the semiclassical error is still small. Note that this difficulty is a peculiarity of the quartic potential. Because of the scale invariance there is no intrinsic system parameter for a semiclassical expansion. We have chosen to implement the method for a rather "difficult" case. In more "molecular" potentials the existence of a harmonic minimum will make the semiclassical method work much better.

In Fig. 2 we have depicted the exact and semiclassical free energies as functions of β for the A_1 and E representations. While for small β all states contribute to the sum (6), the exact free energy saturates at low temperature since only the ground state contributes. In contrast, as mentioned above, the semiclassical approximation leads to a temperature dependent free energy $F_{\mathrm{sc}}(\beta)$ also for large β. Hence we estimate the energies from a point where the corresponding $F_{\mathrm{sc}}(\beta)$ is minimally sensitive to variations in β, i.e., where $dF_{\mathrm{sc}}(\beta)/d\beta$ is minimal. The assumption that thermal errors at those points are small is checked later self-consistently. We note that a similar criterion was first suggested by Stevenson [13] as a "principle of minimal sensitivity" (PMS) in perturbative expansions in quantum field theories and was extensively studied in the past decade [14].

Accordingly, the semiclassical ground state energy for A_1 is estimated from the point where the slope of the semiclassical free energy vanishes, in this case at the maximum $F_{\mathrm{sc}}(\beta_0) = 0.486$ with $\beta_0 = 2.64$. For the E representation, the semiclassical free energy has no maximum but an inflection point at $\beta_0 = 2.41$ so that the minimum of $dF_{\mathrm{sc}}(\beta)/d\beta$ coincides with $d^2F_{\mathrm{sc}}(\beta)/d\beta^2 = 0$. Proceeding along these lines as described above, we obtain the lowest three eigenvalues for each of the five representations from *either* a maximum *or* an inflection point of $F_{\mathrm{sc}}(\beta)$ (see Table I). Despite the difficulties with the scale invariant model, the first two states are found in excellent agreement with the exact eigenvalues with typical errors of 1%. For the second excited states the largest deviations are about 10%. The exact results were obtained by a numerical solution of the Schrödinger equation. In principle, we can go on, but at this simple stage of the procedure one cannot expect reasonable results for more than the first few eigenvalues in each representation due to an accumulation of errors. An improvement of the method that corrects for thermal errors will be presented elsewhere.

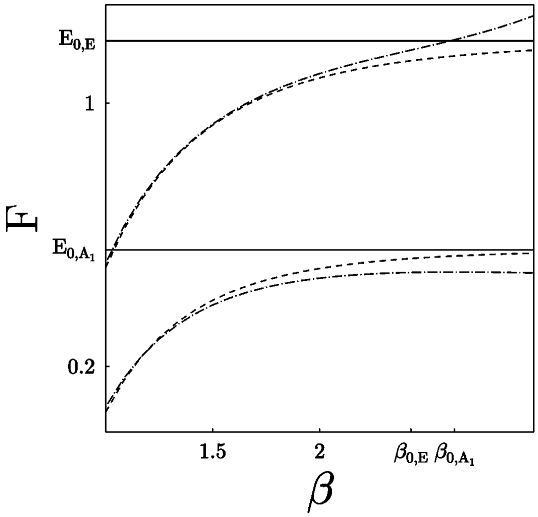

FIG. 2. Free energies for the A_1 (lower curves) and E (upper curves) representations. Dashed lines denote the exact values and dotted-dashed lines the semiclassical values. Solid lines indicate the exact ground state energies.

Given the energy eigenvalues we are able to extract the densities $|\psi_i(\mathbf{x})|^2$ from the density matrix (2) as described above. As shown in Fig. 3, we find excellent agreement with the numerically exact densities. Since the minor differences between semiclassical and exact densities are not apparent in $2d$ contour plots, Fig. 3 shows also integrated densities $d(x)$, integrated along the y axis. In

TABLE I. Semiclassical and exact energy eigenvalues for each of the five representations of the quartic oscillator (4).

$g\backslash n$	0		1		2	
	ex.	sc.	ex.	sc.	ex.	sc.
A_1	0.554	0.486	1.758	1.808	2.493	2.141
A_2	4.037	3.965	5.736	5.647	7.110	6.670
B_1	1.528	1.499	2.376	2.147	3.072	3.086
B_2	2.506	2.442	4.637	4.579	5.886	5.293
E	1.189	1.159	2.047	1.911	2.750	2.381

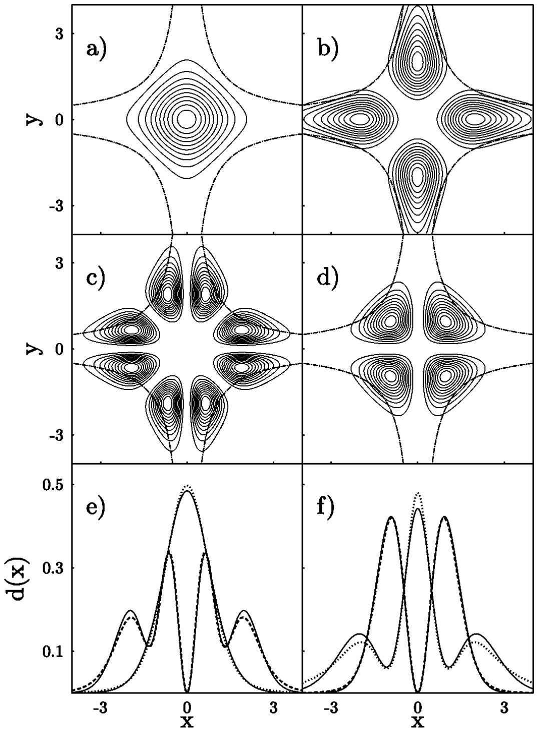

FIG. 3. Semiclassical densities $|\psi_0(\mathbf{x})|^2$ for the (a) A_1, (b) B_1, (c) A_2, and (d) B_2 representations. Semiclassical densities integrated along the y axis for the (e) A_1 (dotted line), A_2 (dashed line), and (f) B_1 (dotted line), B_2 (dashed line) representations are compared with the exact densities (solid lines).

particular, we find that bifurcations of classical paths and the concomitant breakdown of the simple semiclassical density matrix (3) occur in regions in configuration space where the densities are always negligibly small.

In conclusion, we have demonstrated that semiclassical quantization of the equilibrium density matrix is a viable alternative to the real time semiclassical theory. In contrast to real time semiclassical methods, periodic orbits do not play any special role. It is straightforward to apply the method to systems with more than two degrees of freedom. The peeling method allows for determination of the lowest eigenvalues where traditionally semiclassical estimates should be the worst because of the low density of states. We have demonstrated the procedure in detail for the case of a classically chaotic two-dimensional quartic oscillator and found good agreement between the semiclassical and numerically exact lowest eigenvalues and densities.

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