Invariant Tori and Heisenberg Matrix Mechanics: A New Window on the Quantum-Classical Correspondence

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Despite the seminal connection between classical multiply periodic motion and Heisenberg matrix mechanics, we show that there are fundamental, previously undisclosed aspects of this quantum-classical correspondence. These include a quantum variational principle that implies the classical variational principle for invariant tori and the connection between commutation relations and quantization of action variables. Possible applications are described briefly.

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Though applications of great interest (and increasing complexity) continue to be developed, e.g., [1,2], the theory of the semiclassical quantization of invariant tori, using Einstein-Brillouin-Keller (EBK) quantization conditions, appears to be a closed (or at least quiescent) sector in the study of the relationship between the quantum mechanics and the classical mechanics of bound nonseparable systems (for a review, see [3]). The goal of this Letter is to show, nevertheless, that some fundamental aspects of the relationship between quantum mechanics (in the Heisenberg form) and a form of semiclassical mechanics due primarily to Percival and Pomphrey [4–7] (see also [8]) have been overlooked. In the exposition that follows we have tried to be alert to the fact that neither formalism is as widely known as (perhaps) it deserves to be. Although Percival's formulation has been applied extensively and with considerable success to problems in molecular physics [3], it receives only brief mention in the recent books on chaotic dynamics [9]. The associated quantum method, though more than three decades old [10], is mainly known within the context of the nuclear many-body problem [11]. Therefore it is appropriate to start with brief accounts of these two methods. Then follows our main thrust, the derivation of Percival's method from the appropriate quantum formalism. Space permits us to emphasize only the conceptual aspects of this relationship. Nevertheless, there exist intriguing possibilities for applications that we discuss briefly at the end of the account.

We start, therefore, with Percival's scheme. For definiteness, consider a system described by coordinates $x_i, i = 1,\ldots,N$, $\mathbf{x} = (x_1,\ldots,x_N)$, and the Lagrangian

$$L = \sum_i \frac{1}{2}\dot{x}_i^2 - V(\mathbf{x}). \tag{1}$$

For motions that are multiply periodic (on an invariant torus), the coordinates may be expanded in Fourier series,

$$x_i = \sum_{\mathbf{k}} x_{i,\mathbf{k}}(\mathbf{I})\exp(i\mathbf{k}\cdot\boldsymbol{\theta}), \tag{2}$$

where $\boldsymbol{\theta}$ and $\mathbf{I}$ are vectors representing the N angle variables and their corresponding action variables. The equations of motion for the Fourier coefficients,

$$(\boldsymbol{\omega}\cdot\mathbf{k})^2 x_{i,\mathbf{k}} = \partial\langle V\rangle/\partial x_{i,-\mathbf{k}} \equiv F_{i,\mathbf{k}}, \tag{3}$$

can be derived from the variational principle

$$\partial\langle L\rangle/\partial x_{i,-\mathbf{k}} = 0. \tag{4}$$

Here $\boldsymbol{\omega} = (d\boldsymbol{\theta}/dt)$ is the frequency vector, and angular brackets indicate a phase average of the enclosed dynamical variable, i.e., the constant term in its Fourier series. In carrying through this variation, the frequencies are held fixed. Classically, Eq. (3) can serve as the basis for systematic perturbation theory or can be solved nonperturbatively for a finite subset of the amplitudes $x_{i,\mathbf{k}}$, as functions of the frequency vector $\boldsymbol{\omega}$. To quantize the system, we adjoin the EBK quantization conditions in a special form (also $\hbar = 1$),

$$I_j = \sum_i \langle \dot{x}_i(\partial x_i/\partial\theta_j)\rangle = (n_j + \tfrac{1}{4}\alpha_j), \tag{5}$$

where n_j is an integer comprising the components of a vector $\mathbf{n}$, and α_j the associated Maslov index, usually equal to 2 for a vibrational degree of freedom. The frequencies and the energy $E(\mathbf{n}) = \langle H\rangle$ are now determined as functions of $\mathbf{n}$. We emphasize that the approach just described (there are alternatives based on Hamilton's equations) represents a complete method for the study of bound, nearly integrable systems in classical mechanics and in semiclassical quantum mechanics.

Next, we describe the natural quantum progenitor [10,12,13] of the formulation associated with Eqs. (4) and (5). In the following, we emphasize two aspects of this quantum formulation. The first is that the quantum mechanics of bound systems can be studied on the basis of the pairs of equations, describing the dynamics and the kinematics, respectively,

$$[[x_i,H],H] = (\partial V/\partial x_i) \equiv F_i, \tag{6}$$

$$[x_i,[H,x_i]] = 1, \tag{7}$$

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where the Heisenberg equation of motion $p_i = \dot{x}_i = -i[x_i, H]$ has been utilized to eliminate momenta and time derivatives. A scheme for calculating matrix elements and energy differences, whose salient features will now be described (see also Ref. [12]), utilizes the energy-diagonal representation $|\mathbf{n}\rangle$, where $H|\mathbf{n}\rangle = E(\mathbf{n})|\mathbf{n}\rangle$. The equations of motion (6) are applied for arbitrary matrix elements, but only *diagonal* elements of the commutator (7) need be included, as we shall demonstrate later during the discussion of the quantum-classical correspondence. The notation implies that we are confining our attention to systems for which the bound states can be characterized by a set of integers equal in number to the number of degrees of freedom of the system (invariant tori). In evaluating matrix elements of the (nonlinear) force term in the equations of motion, we make use of the completeness relation,

$$\langle \mathbf{n}|AB|\mathbf{n}'\rangle = \sum_{\mathbf{n}''} \langle \mathbf{n}|A|\mathbf{n}''\rangle \langle \mathbf{n}''|B|\mathbf{n}'\rangle , \tag{8}$$

where in the simplest cases both A and B are components of $\mathbf{x}$, though more general functions of the coordinates can be handled [14]. A useful algorithm results when the sum over intermediate states $|\mathbf{n}''\rangle$ converges sufficiently rapidly. Either starting from the ground state $|\mathbf{0}\rangle$ and "working one's way up" in $\mathbf{n}$ values, or else starting from some reference state $|\mathbf{n}\rangle$ and working both up and down, provided one introduces suitable closure approximations to cut off the sums (discussed more fully below in the proof of the quantum-classical correspondence), one can derive a set of nonlinear algebraic equations for the determination of a corresponding number of matrix elements $\langle \mathbf{n}|x_i|\mathbf{n} \pm \mathbf{k}\rangle$ and elementary energy differences, $E(\mathbf{n} + \mathbf{1}_i) - E(\mathbf{n})$, where $\mathbf{1}_i$ is the ith unit vector in the space of $\mathbf{n}$ vectors. From these results, the matrix elements of any other operator, in particular, the energy, can be computed.

We have actually alluded above to two different quantum schemes. The one that calculates from the ground state up is fully quantum and is unrelated to any semiclassical approximation. The second, which builds a calculation about a reference excited state, is the one that can be the starting point for a semiclassical approximation, that therefore enters into the quantum-classical correspondence arguments given below.

The second aspect of the quantum scheme that we wish to emphasize is that the equations of motion (6) can be derived from a quantum variational principle. Consider the functional [15]

$$\begin{aligned} G &= -\mathrm{Tr}L \\ &= \mathrm{Tr}\left\{-\frac{1}{2}\sum_i [x_i, H][H, x_i] + V(\mathbf{x})\right\}. \end{aligned} \tag{9}$$

Though formally extended over all states, in practice the trace is restricted to a finite sum, as described above. The equation of motion (6) follows from the variational principle,

$$\partial G/\partial \langle \mathbf{n}|x_i|\mathbf{n}'\rangle = 0 , \tag{10}$$

when the energy differences that enter in the evaluation of (9) are held fixed.

We are finally in a position to present the crux of this Letter, namely, the arguments that lead from the appropriate one of the quantum schemes just described to the semiclassical quantization scheme previously reviewed. Here we shall use the correspondence principle in a form, differing from that introduced in the first days of quantum mechanics, that has been recognized [3,8,16] as appropriate to obtain semiclassical rather than purely classical accuracy. For example, if A is a real Hermitian operator, we associate the Fourier coefficients in the expansion corresponding to (2) with a displaced matrix element according to the equation

$$A_{\mathbf{k}}(\mathbf{n}) = A_{-\mathbf{k}}(\mathbf{n}) = \langle \mathbf{n} - \tfrac{1}{2}\mathbf{k}|A|\mathbf{n} + \tfrac{1}{2}\mathbf{k}\rangle , \tag{11}$$

and associate the classical frequencies with correspondingly displaced energy differences,

$$\begin{aligned} \omega_i(\mathbf{n}) = {} & E(n_1, \ldots, n_i + \tfrac{1}{2}, \ldots) \\ & - E(n_1, \ldots, n_i - \tfrac{1}{2}, \ldots) . \end{aligned} \tag{12}$$

To study the limit for the dynamics, it is sufficient to confine our attention to the variational principle (10). In the evaluation of $\langle \mathbf{n}|L|\mathbf{n}\rangle$, we expand every matrix element and energy difference encountered in a Taylor series about the reference values just defined. Because of the symmetrical choices made for these reference values, we find the result

$$\langle \mathbf{n}|L|\mathbf{n}\rangle = \langle L\rangle [1 + O(n)^{-2}] . \tag{13}$$

To be explicit, in the evaluation of $\langle \mathbf{n}|L|\mathbf{n}\rangle$, we encounter, typically, a matrix element (switching, for convenience, to a one-dimensional notation)

$$\begin{aligned} \langle n + k_1|A|n + k_1 + k_2\rangle = {} & \langle n - \tfrac{1}{2}k_2|A|n + \tfrac{1}{2}k_2\rangle \\ & + \left(k_1 + \frac{1}{2}k_2\right)\frac{dA_k(n)}{dn} + \cdots . \end{aligned} \tag{14}$$

For this expansion to converge requires that the Fourier series for the dynamical variables converge sufficiently rapidly that k_1 and k_2 can be taken as small compared to n. The series (14) can be then considered as an expansion in $1/n$, since each derivative brings in a power of $1/n$ (one may think of how harmonic oscillator matrix elements grow with n, but the result stated is quite general). The assertion in (13) is that in consequence of the choice made above for the quantum-classical correspondence the error is of order $(1/n)^2$. Because in the expansion (14), all matrix elements are referred to a fixed value of n, the phase averaged quantity $\langle L\rangle$ depends only on this value, and the trace thus becomes a decoupled sum, one term for each state. The convenience of a variational formulation of the equations of motion

is that the result (13) summarizes the quantum-classical correspondence for the dynamics.

The argument just given in relation to Eq. (14) also allows us to emphasize the difference between semiclassical and quantum approximations. In a quantum calculation, k_2 plays a role of Fourier index, the same as in the semiclassical approximation. However, taking n as the reference value, k_1 appears as an n-mixing or bandwidth index. This means that the matrix element exhibited is sharply peaked in k_2 but slowly varying in k_1, and therefore the two dependencies should be treated differently. It is our uniform experience with many different types of applications [11] that this slow dependence precludes the omission of some matrix elements that by their presence render the system of equations overdetermined. The way out of this dilemma is to use the physics of each application to relate the values of the supernumerary elements to those within the chosen subset. In our problem, this is particularly straightforward, since if the maximum value of k_1 in a given approximation is K_1 a simple closure approximation for the quantum case, valid, according to previous arguments, for large n, is

$$\langle n + k_1|A|n + k_1 + k_2\rangle \approx \langle n + K_1|A|n + K_1 + k_2\rangle, \quad k_1 \geq K_1 . \tag{15}$$

In summary, a semiclassical approximation is fully determined by specifying a maximum Fourier component. A quantum approximation has a second parameter, the bandwidth, that, roughly speaking, provides a multiplicative factor for the number of variables and also requires a closure approximation. Without being able to supply further details, we emphasize again that there are actually two quantum methods. One, not related to the semiclassical approximation, builds from the ground state. A second, valid for large quantum numbers, depends on the semiclassical approximation as the starting point. Both are designed to improve on the accuracy of the latter.

There remains the question of the relationship between the commutation relations (7) and the EBK quantization conditions (5) [17]. It is necessary that such a relationship exist, but since the commutation relations are more general than the EBK quantization conditions, just as for the dynamics, the discussion must be tied to the existence of invariant tori. Our solution follows the route, commutation relations $\rightarrow$ Poisson brackets $\rightarrow$ Lagrange brackets $\rightarrow$ EBK conditions. We outline the procedure. (i) The first step is to show that the Fourier series (2) for x_i and the corresponding series for $p_i = \dot{x}_i$ represent a canonical transformation from the original canonical variables $\mathbf{x}, \mathbf{p}$ to the new set $\boldsymbol{\theta}, \mathbf{I}$, i.e., we must show that these series satisfy the Poisson bracket (PB) relations. But the diagonal elements of the commutation relations (7), all that were required to be satisfied in the quantum scheme, have as their classical limit only the phase average of the corresponding PB relation. We must prove that all remaining Fourier coefficients of this relation and the complete Fourier series of all other PB relations vanish identically. Toward this end, the first step is to show that all fundamental commutators are constants of the motion, i.e., that their time derivatives vanish in consequence of the equations of motion. This is an elementary exercise, requiring only, in addition to the equations of motion, the Jacobi identity satisfied by the commutator bracket. This means, of course, that the vanishing of all off-diagonal elements of the commutators is a dynamical consequence of the equations of motion. A second step is to recognize that all diagonal elements other than the one utilized in the algorithm vanish from simple symmetry relations. Finally, the diagonal elements in the calculational scheme are determined to have their correct values. The classical limit of the totality of these assertions constitutes the necessary statements about PB relations and constitutes a proof that the series (2) and the corresponding one for the momenta define a canonical transformation to action-angle variables. At the same time, the quantum considerations in the above demonstration provide the promised justification for our choice of kinematical conditions in the quantum scheme, since what has been shown is that these are the only nontrivial kinematical conditions that are not, in fact, a consequence of the dynamics. (ii) The next step is to remember [18] that the array of PB relations and an associated set of Lagrange bracket relations are reciprocal matrices in phase space, one set therefore implying the other. But it is not difficult to demonstrate *from the Percival form* (5) that a typical EBK quantization condition is an integrated form of the phase average of the Lagrange bracket between θ_i and I_i. The integration constant, which is the Maslov index, will be determined both by the commutation relations and the geometrical properties of the canonical variables on a case by case basis. This completes our discussion of the quantum-classical correspondence.

We add some brief remarks about possible applications. The listing and discussion, far from exhaustive, will be limited to three high-priority topics.

(1) A semiclassical application.—In the literature of atomic physics [1] and of chemical physics [3], Percival's and related methods are perceived of as quite distinct from another powerful approach to semiclassical quantization, the Birkhoff-Gustavson (BG) method [19]. In the latter one carries out algebraically a series of perturbative canonical transformations in order to express the Hamiltonian as far as possible as a polynomial in action variables, which is then quantized. Since any nonperturbative solution of Percival's equations is exact to a known order of perturbation theory (and involves a selective summation of higher order contributions), it is intuitively clear that it should be possible to construct a BG type solution directly from a Percival solution. This possibility, which remains to be implemented, has been overlooked in the literature.

(2) Quantization scheme for invariant tori.—With only a modest increase in computational effort, it is feasible to apply the method of Heisenberg matrix mechanics described in this Letter to the same class of problems for which the application of semiclassical approximations have hitherto been successful. [As noted after Eq. (15), there are actually two different quantum approximation methods.] Such applications will be reported in a more complete publication.

(3) Quantization of classically chaotic systems.—The study of bound quantum systems associated with classically chaotic motion has usually been based on diagonalization of the Hamiltonian in a convenient and often large basis of states. It would be of interest if we could replace the large-basis linear calculation by a small basis nonlinear one. Consider a two-dimensional system and suppose it to possess only bound states. (In any event we use a notation with discrete labels only.) We make no assumption concerning the existence of invariant tori, but simply order the energy levels of the system with coordinates x, y, in a linear sequence, $N = 0, 1, \ldots$. A calculation can be based on the equations (with corresponding equations for the coordinate y)

$$(E_{N'} - E_N)^2 x_{NN'} = -(F_x)_{NN'}, \tag{16}$$

$$\sum_{N'} (E_{N'} - E_N)|x_{NN'}|^2 = 1, \tag{17}$$

where E_N are the exact eigenvalues. These equations can be viewed in two ways, either as a set of sum rules to be satisfied by the exact solutions of the quantum mechanical problem, found by some other means such as matrix diagonalization in a basis, or else as the foundation for a computational scheme generalizing the schemes described for invariant tori. By summing the commutation relation from 0 to N, we can replace (17) by the positive sum (with a corresponding equation for y),

$$\sum_{N'=N+1}^{\infty} \sum_{N''=0}^{N} (E_{N'} - E_{N''})|x_{N''N'}|^2 = N + 1. \tag{18}$$

These relations are interesting because they guarantee the convergence of certain sums, and thus imply that the matrix elements cannot spread out too far as a function of energy differences. The utility of this observation remains to be demonstrated, but imparts some measure of optimism concerning the application of this formalism.

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[1] H. Hasegawa, M. Robnik, and G. Wunner, Prog. Theor. Phys. Suppl. **98**, 198 (1989).
[2] J. Müller, J. Burgdörfer, and D. Noid, Phys. Rev. A **45**, 1471 (1992).
[3] G. S. Ezra, C. C. Martens, and L. E. Fried, J. Phys. Chem. **91**, 3721 (1987).
[4] I. C. Percival, J. Phys. A **7**, 794 (1974).
[5] I. C. Percival and N. Pomphrey, Mol. Phys. **35**, 649 (1978).
[6] I. C. Percival, Adv. Chem. Phys. **36**, 1 (1977).
[7] I. C. Percival, J. Phys. A **12**, L57 (1979).
[8] A. Klein and C. T. Li, J. Math. Phys. **20**, 572 (1979).
[9] The longest account of which we are aware is a summary of one paragraph in A. J. Lichtenberg and M. A. Lieberman, *Regular and Chaotic Dynamics* (Springer, New York, 1993), 2nd ed., p. 249. Nevertheless, it was this reference that rekindled the authors' interest in the topic of this Letter.
[10] A. K. Kerman and A. Klein, Phys. Rev. **132**, 1326 (1963).
[11] *Nuclear Structure Studies,* edited by R. Bengtsson, J. Draayer, and W. Nazarewicz (World Scientific, Singapore, 1992), p. 229.
[12] C. T. Li, A. Klein, and F. R. Krejs, Phys. Rev. D **12**, 2311 (1975).
[13] A. Klein, C. T. Li, and M. Vassanji, J. Math. Phys. **21**, 2521 (1980).
[14] C. T. Li and A. Klein, Fizika **22**, 67 (1990).
[15] This form of the variational principle is the final one of several versions derived, e.g., in [14]. A related variational principle was introduced by M. Born and P. Jordan, Z. Phys. **34**, 858 (1925), but never recurs in later work.
[16] C. Jaffé and F. L. Roberts, in *Quantum Dynamics of Chaotic Systems,* edited by J.-M. Yuan, D. H. Feng, and G. M. Zaslovsky (Gordon and Breach, New York, 1992), p. 177.
[17] The problem of showing that all the commutation relations are constants of the motion, which constitutes the initial part of the demonstration described below, is mentioned but not solved in M. Born, W. Heisenberg, and P. Jordan, Zeit. f. Phys. **35**, 557 (1926).
[18] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, 1980), second ed., p. 402.
[19] F. G. Gustavson, Astrophys. J. **71**, 670 (1966).