Solutional method for the energies of a parameter-dependent system

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It is shown that the functional form for the energies of a parameter-dependent system can be found by minimizing an associated semiclassical energy function in configuration space.

Consider the Hamiltonian for a system of n coupled oscillators,

$$H=\sum_{i=1}^{n}\left(-\frac{\partial^2}{\partial q_i^2}+\xi_i q_i^2\right)+\sum_{i,j=1}^{n}\gamma_{ij}q_i^2q_j^2, \quad (1)$$

where the real constant ξ_i are positive or negative and the $\gamma_{ij}\equiv\gamma_{ji}$ constitute a positive-definite array. From the virial theorem for an energy eigenstate

$$\sum_{i=1}^{n}\left(\left\langle\frac{\partial^2}{\partial q_i^2}\right\rangle+\xi_i\langle q_i^2\rangle\right)+2\sum_{i,j=1}^{n}\gamma_{ij}\langle q_i^2q_j^2\rangle=0, \quad (2)$$

and the Hellmann-Feynman equations

$$\frac{\partial E}{\partial\xi_i}=\langle q_i^2\rangle, \quad \frac{\partial E}{\partial\gamma_{ij}}=\langle q_i^2q_j^2\rangle, \quad (3)$$

it follows that the energy $E\equiv\langle H\rangle$ satisfies the Euler homogeneity equation

$$E=2\sum_{i=1}^{n}\xi_i\frac{\partial E}{\partial\xi_i}+3\sum_{i,j=1}^{n}\gamma_{ij}\frac{\partial E}{\partial\gamma_{ij}}. \quad (4)$$

Implying that

$$E(\xi,\gamma)\equiv\mu^{-1}E(\mu^2\xi,\mu^3\gamma)$$

for all real $\mu>0$, (4) is insufficient by itself to determine the entire functional dependence of E on the parameters ξ_i and γ_{ij}. However, as indicated by the recent work of Orland,[1] (4) can be supplemented by the approximate conditions

$$\frac{\partial E}{\partial\xi_i}\frac{\partial E}{\partial\xi_j}=\frac{\partial E}{\partial\gamma_{ij}} \quad (5)$$

which follow from (3) and the semiclassical relation $\langle q_i^2q_j^2\rangle\cong\langle q_i^2\rangle\langle q_j^2\rangle$; in view of Orland's results for the $n=1$ case, the regime for approximate validity of (5) (spanned by the parameters ξ_i, γ_{ij}, and the quantum numbers of the energy eigenstates) can be expected to transcend the regime of the latter semiclassical relation if E is required to satisfy Eq. (4). There remains the task of solving $\frac{1}{2}(n^2+n)$ nonlinear equations (5) in combination with (4) to determine the parameter dependence featured by E.

My rigorous mathematical result is the following: A solution to (4) and (5) obtains as

$$E=\min_{\vec{q}}\tilde{E}(\vec{q}), \quad (6)$$

$$\tilde{E}(\vec{q})\equiv 2A\left(\sum_{i=1}^{n}q_i^2\right)^{-1}+\sum_{i=1}^{n}\xi_iq_i^2+\sum_{i,j=1}^{n}\gamma_{ij}q_i^2q_j^2, \quad (7)$$

in which A is an absolute constant (depending on the quantum numbers of the energy eigenstate but not on the ξ_i's or γ_{ij}'s). The intuitive basis for this result resides in the fact that the kinetic-energy operator in (1) acts roughly like a repulsive $\|\vec{q}\|^{-2}$ term on bound-state wave functions.[2] I was led to consider the possibility that (6) satisfies both (4) and (5) because only the homogeneity order in $\vec{q}$ (and not the differential operator structure) of the kinetic energy enters in its virial-theorem elimination from E, effected above by (2).

Proof of (6). The minimum value of (7) is at

$$q_i^2=\sum_{j=1}^{n}\gamma_{ij}^{-1}(A\phi^2-\tfrac{1}{2}\xi_j) \quad (8)$$

where γ_{ij}^{-1} is the positive-definite symmetric array inverse to γ_{ij} and the reciprocal norm squared of $\vec{q}$ is denoted by

$$\phi\equiv\left(\sum_{i=1}^{n}q_i^2\right)^{-1}. \quad (9)$$

By summing (8) over i, one obtains the cubic equation for ϕ

$$A\left(\sum_{i,j=1}^{n}\gamma_{ij}^{-1}\right)\phi^3-\frac{1}{2}\left(\sum_{i,j=1}^{n}\gamma_{ij}^{-1}\xi_j\right)\phi=1 \quad (10)$$

with a unique positive root.[3] The substitution of (8) into (7) yields (6) as

$$E=3A\phi+\tfrac{1}{2}A\sum_{i,j=1}^{n}\gamma_{ij}^{-1}\xi_j\,\phi^2-\frac{1}{4}\sum_{i,j=1}^{n}\gamma_{ij}^{-1}\xi_i\xi_j. \quad (11)$$

Differentiating both (10) and (11) with respect to ξ_i and eliminating $\partial\phi/\partial\xi_i$ between the resulting equations produces

$$\frac{\partial E}{\partial\xi_i}=A\phi^2u_i-v_i, \quad (12)$$

with the definitions

$$u_i\equiv\sum_{j=1}^{n}\gamma_{ij}^{-1}, \quad v_i\equiv\frac{1}{2}\sum_{j=1}^{n}\gamma_{ij}^{-1}\xi_j. \quad (13)$$

Similarly, by differentiating (10) and (11) with respect to γ_{ij}, making use of the formula

$$\frac{\partial\gamma_{kl}^{-1}}{\partial\gamma_{ij}}=-\tfrac{1}{2}[\gamma_{ik}^{-1}\gamma_{jl}^{-1}+(i\longleftrightarrow j)]\,,$$

and eliminating $\partial\phi/\partial\gamma_{ij}$ between the resulting equations, one obtains

$$\frac{\partial E}{\partial\gamma_{ij}}=A^2\phi^4u_iu_j-A\phi^2(u_iv_j+u_jv_i)+v_iv_j\,. \qquad (14)$$

It is easily verified that the right-hand side of (4) reproduces (11) after substitution of (12) and (14). Moreover, the latter formulas for the derivatives of E satisfy (5). Hence, a solution to (4) and (5) is given by (6), or more explicitly, by (11) with (10).

Remarks. For $n=1$ my solution reduces immediately to that of Orland,[1] with $\xi_1\equiv 1$, $\gamma_{11}\equiv z$ and ϕ in (10) and (11) replaced by Orland's p. I have introduced the constant A in (7) to be precisely the A which appears in Orland's $n=1$ solution [hence the irrelevant prefactor of 2 in (7)]. For higher-dimensional systems with $n>1$, my solution to (4) and (5) is a member of a one-parameter family of solutions obtainable from (6) by modifying the kinetic-energy term in (7); in place of the reciprocal norm squared (9), an expression of the form

$$\left(\sum_{i=1}^{n}|q_i|^{2\lambda}\right)^{-1/\lambda}$$

for all real $\lambda\neq 0$ yields a member of the family of solutions. In particular, the kinetic-energy representation with $\lambda=-1$ is clearly required by a system of uncoupled oscillators with the array (γ_{ij}) diagonal. Because it retains the configuration-space rotation symmetry of the kinetic-energy operator in (1), the $\lambda=+1$ choice employed in (7) is indicated on physical grounds for the most interesting cases of essential (strong) coupling.[4] Then the dependence on ξ_i and γ_{ij} is contained exclusively in the permutation-symmetric summations involving γ_{ij}^{-1} in (10) and (11).

By minimizing associated semiclassical energy functions like (7), the functional form for the energies of other parameter-dependent systems can be found and shown to satisfy exact and approximate equations similar to (4) and (5) in the example presented here.

ACKNOWLEDGMENT

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[1] H. Orland, Phys. Rev. Lett. 42, 285 (1979); for an antecedent of the method see G. Rosen, Phys. Rev. D 1, 2880 (1970).

[2] See, for example, R. P. Feynman, R. B. Leighton, and M. Sands, *Lectures on Physics* (Addison-Wesley, Reading, Mass., 1963), Vol. III, pp. 2–6; for this uncertainty-principle representation to have approximate validity, the wave function must be confined to a connected region about $\vec{q}=0$ [E. H. Lieb, Rev. Mod. Phys. 48, 553 (1976)].

[3] Putting

$$\Lambda\equiv\left(6A\sum_{i,j=1}^{n}\gamma_{ij}^{-1}\right)^{1/2}\quad\text{and}\quad\Omega\equiv\left(\sum_{i,j=1}^{n}\gamma_{ij}^{-1}\xi_j\right)^{1/2},$$

one obtains

$$\phi=2\,\Omega\Lambda^{-1}\cosh[\tfrac{1}{3}\cosh^{-1}(3\Lambda\Omega^{-3})]$$

for strong anharmonic coupling with $\Omega^3\leq 3\Lambda$; the functions cosh and $\cosh^{-1}$ go into cos and $\cos^{-1}$ in this formula for $\Omega^3\geq 3\Lambda$.

[4] Systems with weak or partial coupling may be characterized more accurately by λ values in the intermediate range $-1<\lambda<1$. For any specific system this matter can be elucidated by estimating the ground-state energy via an alternative analytical procedure. One such procedure is to use the Sobolev inequality [G. Talenti, Ann. Mat. Pura Appl. 110, 353 (1976); G. Rosen, SIAM J. Appl. Math. 21, 30 (1971)] for $n\geq 3$:

$$\sum_{i=1}^{n}\int\left|\frac{\partial\psi}{\partial q_i}\right|^2 d^nq\geq\tau_n[\psi]$$
$$\equiv 2^{-2+2/n}\pi^{1+1/n}(n^2-2n)\left[\Gamma\left(\frac{n+1}{2}\right)\right]^{-2/n}\times\left(\int|\psi|^{2n/(n-2)}d^nq\right)^{1-2/n}$$

in combination with the ground-state estimation method of Lieb (see Ref. 2, p. 555). By evaluating the right-hand side of

$$E_0\geq\min_{\psi}\left(\tau_n[\psi]+\int|\psi|^2V(q)\,d^nq\right)\Big/\int|\psi|^2d^nq,$$

one obtains the tight lower bound on the ground-state energy $E_0\geq\hat{E}_0$, where $\hat{E}_0$ is given implicitly by

$$\int_S[\hat{E}_0-V(q)]^{n/2}d^nq=2^{1-n}\pi^{(n+1)/2}(n^2-2n)^{n/2}\left[\Gamma\left(\frac{n+1}{2}\right)\right]^{-1},$$

$$S\equiv\{q:V(q)\leq\hat{E}_0\}\,.$$