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Energies of Parameter-Dependent Systems

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The energy of a linearly perturbed system is shown to verify a nonlinear first-order differential equation in the semiclassical limit. Solutions of this equation are compared to the exact energies, for a quartic oscillator.

Let us consider a perturbed Hamiltonian

$$H(z)=p^2+v(x)+zw(x), \tag{1}$$

where $p^2=-d^2/dx^2$, and the perturbation depends linearly on a parameter z.

There has been considerable interest in determining the dependence of the energy of such a sys-system as a function of z.[1] In particular, analyticity and crossing[2] problems are very important.

Let us denote by $E(z)$ an eigenvalue of the Hamiltonian

$$H(z)\,|\,\psi(z)\rangle=E(z)|\,\psi(z)\rangle, \tag{2}$$

where $E(z)$ is the envelope of a one-parameter family of straight lines, namely the tangents to $E(z)$, which satisfy the equation

$$f_{\psi(z_0)}(z)=\frac{\langle\psi(z_0)|\,p^2+v\,|\psi(z_0)\rangle}{\langle\psi(z_0)|\psi(z_0)\rangle}+\frac{\langle\psi(z_0)|w|\psi(z_0)\rangle}{\langle\psi(z_0)|\psi(z_0)\rangle}\,z, \tag{3}$$

where $\psi(z_0)$ is the eigenstate of $H(z_0)$, corresponding to the energy $E(z_0)$.

Therefore, an elementary theorem of geometry[3] states that $E(z)$ verifies a first-order differential equation. It seems then of crucial importance to determine this differential equation. I show, in the next paragraph, how such an equation can be obtained in the classical limit.

We know that

$$E(z)=\langle p^2\rangle+\langle v\rangle+z\langle w\rangle, \tag{4}$$

where the brackets denote mean values in some eigenstate of the Hamiltonian. From the Hellmann-Feynman theorem, we know that

$$\langle w\rangle=dE(z)/dz. \tag{5}$$

In order to obtain a closed differential equation for $E(z)$, one needs to express the quantity $\langle p^2\rangle+\langle v\rangle$ as a function of $dE(z)/dz$, $E(z)$, and z. This can be done, in some approximation, by the use of the virial theorem, which states that

$$2\langle p^2\rangle=\langle x\,\partial v/\partial x\rangle+z\langle x\,\partial w/\partial x\rangle. \tag{6}$$

In general, it is possible to express any function in terms of a given function. Hence I shall make the assumption that it is possible to write

$$x\,\partial v/\partial x=G(w(x)), \tag{7a}$$

$$x\,\partial w/\partial x=F(w(x)), \tag{7b}$$

$$v(x)=K(w(x)). \tag{7c}$$

In the semiclassical limit, we know that

$$\langle A^n(x)\rangle=\langle A(x)\rangle^n. \tag{8}$$

Therefore, in this approximation, Eq. (4) takes

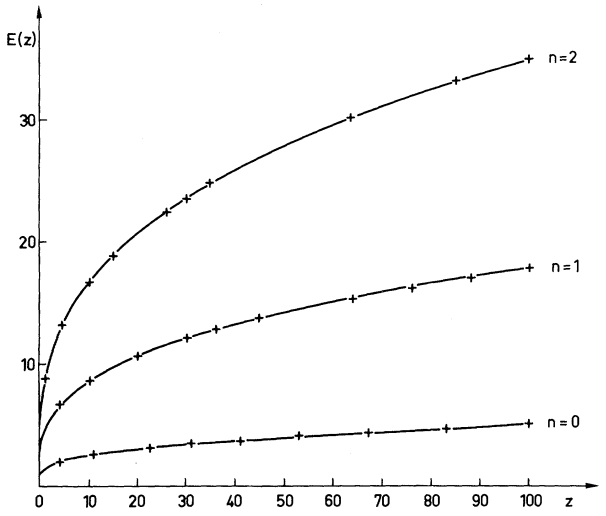

FIG. 1. The energy, as a function of z for the ground state, and the two first excited states: Full line, results of Ref. 4; crosses, our calculations.

the closed form

$$E(z)=z\frac{dE}{dz}+K\left(\frac{dE}{dz}\right)+\tfrac{1}{2}G\left(\frac{dE}{dz}\right)+\frac{z}{2}F\left(\frac{dE}{dz}\right). \tag{9}$$

This equation defines the trajectories of $E(z)$ as a function of z.

I shall make three comments about Eq. (9): (i) It is exact for scale-invariant potentials; namely, for v and w which are homogeneous functions of x, of the same degree. (ii) It becomes exact for large z, and provides the exact behavior of the energy at large z. (iii) The solutions of (9) depend on one constant of integration. From remark (ii), one sees that this constant should be fitted at large z with the exact energies.

I now show an application of this method to the quartic oscillator, with

$$v(x)=x^2, \tag{10a}$$

$$w(x)=x^4. \tag{10b}$$

The solution of (9) can be parametrized as

$$z=Ap^3-0.5p,\quad E(z)=3Ap+0.5/p,\quad p>0. \tag{11}$$

Figure 1 shows a plot of (11), for the first three levels of the quartic oscillator, compared with the exact numerical results of Biswas *et al.* The constant A has been fitted, for all levels, to the energy at $z=100$ given in Ref. 4. For the three

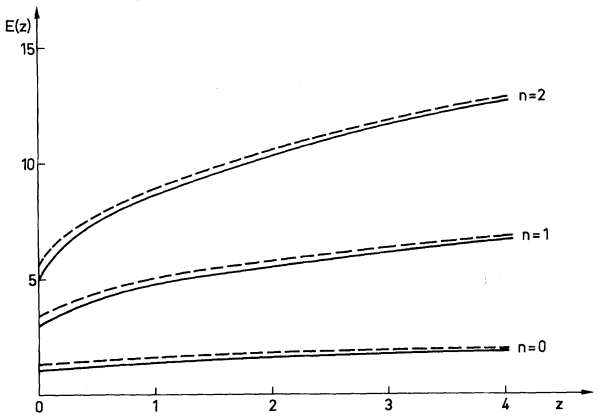

FIG. 2. Same as Fig. 1. Full line, results of Fig. 4; dashed line, our calculations.

first levels, one finds, respectively, $A_0=0.207\,206$, $A_1=1.419\,631$, $A_2=3.905\,864$.

The agreement is strikingly good, for all levels, for values of z larger than 4. For z smaller than 4 (Fig. 2), the agreement is still rather good for the excited states. I note that for z negative, the energy $E(z)$ becomes multivalued, and shows a singularity at $z=0$. This is in accord with the WKB analysis of Bender and Wu[5] and the rigorous results of Simon[6] and confirms the invalidity of application of the perturbation theory around $z=0$.

The method presented here should be valid in a semiclassical limit, namely for large z. Despite the good agreement in the quartic-oscillator example, it would be very interesting to find a systematic way of improving Eq. (8), in order to include higher-order terms in $1/z$.

This whole formalism can easily be extended to the many-body problem, and would be of considerable interest, since it would transform it to a one-variable differential equation. For example, if we take the Hamiltonian

$$H=\sum_{i=1}^{N}\vec{p}_i^{\,2}+\frac{z}{2}\sum_{1\le i\ne j\le N}v(\vec{r}_{ij}), \tag{12}$$

where the two-body potential $v(\vec{r})$ depends only on the modulus of $\vec{r}$, it is easy to see that Eqs. (4), (5), (6), and (9) become

$$E(z)=N\langle\vec{p}_1^{\,2}\rangle+\tfrac{1}{2}zN(N-1)\langle v(\vec{r}_{12})\rangle, \tag{4'}$$

$$dE/dz=\tfrac{1}{2}N(N-1)\langle v(\vec{r}_{12})\rangle, \tag{5'}$$

$$2N\langle\vec{p}_1^{\,2}\rangle=\frac{z}{2}\sum_{1\le i\ne j\le N}\langle\vec{r}_{ij}\cdot\nabla_i v(\vec{r}_{ij})\rangle = z\frac{N(N-1)}{2}\langle\vec{r}_{12}\cdot\nabla_1 v(\vec{r}_{12})\rangle. \tag{6'}$$

By making similar assumptions as in Eqs. (7) and (8), i.e.,

$$\vec{r}\cdot\nabla v(\vec{r}) = F(v(\vec{r})), \tag{7'}$$

one obtains

$$E(z) = \frac{z}{4} N(N-1) F\left(\frac{2}{N(N-1)}\frac{dE}{dz}\right) + z\frac{dE}{dz}. \tag{9'}$$

This very simple equation should be of great use in studying the properties of many-body systems, such as extensivity or saturation.

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Light Scattering from Nonequilibrium Stationary States: The Implication of Broken Time-Reversal Symmetry

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We report a theroetical prediction of a new feature in the spectrum of light scattered from a fluid in a nonequilibrium stationary state with a temperature gradient. The spectrum is not symmetric in the frequency shift and the Brillouin components have different intensities. The phenomenon is linked to the breaking of time-reversal symmetry and to the appearance of a static correlation function between momentum and number densities which is zero in equilibrium, but has a $1/k^2$ dependence in the stationary state. We suggest a light scattering experiment by means of which these predictions can be verified.

We report here some results of a theoretical investigation of nonequilibrium stationary states (NESS) in simple fluids. The theory predicts some new effects and one of the purposes of this communication is to suggest an interesting experiment which can probe the new phenomena.

Our analysis is based on nonlinear response theory. In the context of this theory, we have assumed the existence of a set of "slow" variables, which spans the slow, macroscopic evolution in an N-body system.[1,2] For a simple fluid it is customary to take the densities of the conserved variables (i.e., energy, number, and momentum) to compose this set. In the following we denote such a set by $\underline{A}(X^N(t), \vec{r})$, where X^N is the phase point and $\vec{r}$ is the position in space; we use a shorthand notation and write $\underline{A}(\vec{r}, t)$. The set of conjugate variables is denoted by $\underline{\Phi}(\vec{r})$. An inner product in the space of such sets involves integration over the spatial variables as well as summation on the indices (including Cartesian component indices where appropriate), and will be denoted by $*$, as $\underline{A}(\vec{r}_1, t) * \underline{B}(\vec{r}_1)$.

With this in mind, we have derived the NESS average of an *arbitrary* dynamical variable, say $B(\vec{r}, t)$.[3] Since an isolated system has no NESS we solved the Liouville equation for a system composed of three subsystems, two of which are large and act as reservoirs. The third subsystem is smaller and in it a quasistationary state is established. The result for the NESS average (denoted by $\langle\ \rangle_{NE}$) is[3]

$$\langle B(\vec{r})\rangle_{NE} = \langle B(\vec{r})\rangle_L - \int_0^\infty d\tau \langle \hat{B}(\vec{r})\underline{\hat{I}}(\vec{r}_1, -\tau)\rangle_L * \nabla\beta\underline{\Phi}(\vec{r}_1). \tag{1}$$

In this equation and the following, the caret denotes the deviation of a quantity from its equilibrium average. The notation $\langle\ \rangle_L$ stands for an average on a "local" distribution function

$$f_L(X^N) = \frac{f_{G.C.}(X^N)\exp[\beta\underline{\Phi}(\vec{r}_1) * \underline{A}(\vec{r}_1)]}{\sum_N \int dX^N f_{G.C.}(X^N)\exp[\beta\underline{\Phi}(\vec{r}_1) * \underline{A}(\vec{r}_1)]}, \tag{2}$$

