Quantum chaos and regularity in ultracold Fermi gases

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Quantum fluctuation of the energy is studied for an ultracold gas of interacting fermions trapped in a three-dimensional potential. Periodic-orbit theory is explored, and energy fluctuations are studied versus the particle number for generic regular and chaotic systems, as well as for a system defined by a harmonic confinement potential. Temperature effects on the energy fluctuations are investigated.

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A trapped gas of ultracold fermionic atoms constitutes an exciting quantum mechanical many-body system that presently attracts much attention (see, e.g., [1]). The confinement potential, as well as the atomic two-body interaction, can be experimentally controlled [2], as can the number of atoms in the trap. Due to quantum effects the energy is expected to vary, or fluctuate, in a nonsmooth way as the external parameters are varied. A crucial parameter in the determination of the fluctuations is the dynamics of the system, which may correspond to classical regular or chaotic motion. By using semiclassical methods [3,4] energy fluctuations of the many-body system are calculated for generic (quantum) chaotic and regular systems. We show that a minimum of fluctuations is obtained by making the dynamics chaotic, while a harmonic confinement potential generally gives rise to much larger fluctuations.

The atoms experience an external trapping potential, V_{trap}, and a mutual two-body interaction. For a dilute gas the atom-atom interaction is well approximated by a zero-range delta potential, and the many-body Hamiltonian can be written as

$$H=\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}+V_{\mathrm{trap}}(\mathbf{r}_i)+\frac{4\pi\hbar^2 a}{m}\sum_{i<j}\delta^{(3)}(\mathbf{r}_i-\mathbf{r}_j), \tag{1}$$

where a is the s-wave scattering length for elastic atom-atom collisions that can be experimentally tuned by a magnetic field through a Feshbach resonance [5] from large negative to large positive values. We restrict the present study to positive values of a, i.e., to repulsive interactions between the atoms. In addition, we assume an ultracold gas, implying quantum effects being important. We study a fully unpolarized system consisting of N fermions with two spin states, spin up ($\uparrow$) and spin down ($\downarrow$). The total density is then given by $n(\mathbf{r})=n^{\uparrow}(\mathbf{r})+n^{\downarrow}(\mathbf{r})=2n^{\uparrow}(\mathbf{r})$, where $n^{\uparrow}$ and $n^{\downarrow}$ are the spin-up and spin-down particle densities. From Eq. (1) the single-particle Hartree-Fock equation is obtained as follows:

$$\left[-\frac{\hbar^2}{2m}\Delta+gn^{\uparrow}(\mathbf{r})+V_{\mathrm{trap}}(\mathbf{r})\right]\phi_i^{\downarrow}=\epsilon_i\phi_i^{\downarrow}, \tag{2}$$

where we have introduced the interaction parameter $g=4\pi\hbar^2 a/m$. The effective mean-field potential is thus given by

$$V_{\mathrm{eff}}=gn^{\uparrow}(\mathbf{r})+V_{\mathrm{trap}}(\mathbf{r}). \tag{3}$$

The classical dynamics in this effective potential defines the motion as regular, chaotic, or mixed and we expect different features of the corresponding quantum spectra [6]. The diluteness condition of the gas is fulfilled when $\bar{n}a^3\ll 1$, where $\bar{n}^{-1/3}$ is the mean interparticle spacing.

With given confinement potential and two-body interaction, Eq. (2) can be numerically solved and the total energy calculated for a specified number of atoms (see, e.g., Ref. [7]). In this study we are, however, not interested in a detailed description, but rather in general features of the system, and the role of the underlying dynamics. This can be obtained by utilizing semiclassical methods to calculate the total energy of N confined atoms, $U(N)=\bar{U}+\tilde{U}$, at low temperature. As is usual in semiclassics [8], the total energy is divided into a smoothly varying part, $\bar{U}$, and a fluctuating part, $\tilde{U}$, and we shall focus on the nontrivial fluctuating energy. At low temperatures $k_BT\ll\mu$, where μ is the Fermi energy, the fluctuating part can be calculated to leading order in $\hbar$, as [3]

$$\tilde{U}(N)=2\hbar^2\sum_p\sum_{r=1}^{\infty}\frac{A_{p,r}\kappa_T(r\tau_p)}{r^2\tau_p^2}\cos[rS_p/\hbar+\nu_{p,r}], \tag{4}$$

where the summation p runs over all classical periodic orbits in the effective mean-field potential, and r is their repetitions. The amplitude $A_{p,r}$ depends on the stability of the orbit, $S_p(E)$ is the classical action, $\tau_p=dS_p/dE$ is the period, and $\nu_{p,r}$ is the Maslov index. Temperature effects are included through the function

$$\kappa_T(\tau)=\frac{\tau/\tau_T}{\sinh(\tau/\tau_T)}, \tag{5}$$

where $\tau_T=h/(2\pi^2 k_BT)$. At zero temperature $\kappa_T=1$.

The classical functions in Eq. (4) are evaluated at $E=\mu$. Since Eq. (4) suffers from severe convergence problems, we characterize the fluctuating energy, $\tilde{U}(N)$, by computing its moments. The first nontrivial moment is the variance $\sigma^2=\langle\tilde{U}^2\rangle$ that gives the typical size of the fluctuations. This can be written as [3]

$$\sigma^2 = \frac{\hbar^2}{2\pi^2}\int_0^\infty \frac{K(\tau)}{\tau^4}\kappa_T^2 d\tau, \tag{6}$$

where $K(\tau)$ is the diagonal part of the spectral form factor (the Fourier transform of the two-point energy correlation function). The form factor is by definition system dependent but for long times, i.e., $\tau \gg \tau_{\min}$ ($\tau_{\min}$ is the period of the shortest periodic orbit), general statistical properties can be derived [9,10], namely,

$$K_{\text{reg}} = \tau_H \tag{7}$$

for the regular case, and

$$K_{\text{ch}} = \left[2\tau - \tau \ln\left(1 + \frac{2\tau}{\tau_H}\right)\right]\Theta(\tau_H - \tau) + \left[2\tau_H - \tau \ln\left(\frac{2\tau + \tau_H}{2\tau - \tau_H}\right)\right]\Theta(\tau - \tau_H) \tag{8}$$

for the chaotic case. In these expressions $\tau_H = h\bar{\rho}$ is the Heisenberg time and Θ is the Heaviside step function. The so-called $\tau_{\min}$ approximation assumes the smooth behavior of K [Eqs. (7) and (8)] all the way down to $\tau = \tau_{\min}$; for $\tau < \tau_{\min}$ there are no periodic orbits and the form factor is zero. In this approximation simple expressions can be derived for the energy fluctuations assuming regular or chaotic dynamics, by inserting the corresponding expressions for the form factor into Eq. (6). At temperature zero this gives [3]

$$\sigma_{\text{reg}}^2 = \frac{b}{24\pi^4}E_c^2 \tag{9}$$

for the regular case, where $E_c = h/\tau_{\min}$ and $b = E_c\bar{\rho} = \tau_H/\tau_{\min}$ ("dimensionless conductance"). In the range $\tau_{\min} \ll \tau \ll \tau_H$, and for not too small numbers of particles, it is a good approximation to write $K_{\text{ch}} = 2\tau$. In this approximation the energy fluctuations for chaotic dynamics become

$$\sigma_{\text{ch}}^2 = \frac{1}{8\pi^4}E_c^2. \tag{10}$$

In the studies below we shall, however, generally integrate Eq. (6) numerically. The important parameters to determine the fluctuations in energy are thus the period of the shortest periodic orbit, $\tau_{\min}$, and the mean level spacing at the Fermi energy, $\delta = 1/\bar{\rho} = d\mu/dN$. As the shortest orbit we assume a "diameter orbit," i.e., motion along the diameter in the effective potential, and get $\tau_{\min} = 4\int_0^{R_{\max}} dr/v(r)$, where $v(r)$ is the classical velocity and $R_{\max}$ is the corresponding maximal radius.

At nonzero temperature Eq. (6) is solved numerically using the respective expression for the form factor, Eqs. (7) and (8). In the limit of very low temperature an analytical expression of the energy fluctuations may be derived for the chaotic case ($\tau_T \gg \tau_H \gg \tau_{\min}$) [11],

$$\sigma_{\text{ch}}^2 = \frac{\hbar^2}{2\pi^2}\left[\left(\frac{1}{\tau_{\min}} - \frac{1}{\tau_H}\right)^2 + \frac{1}{3}\left(\frac{1}{\tau_H^2} - \frac{1}{\tau_T^2}\right)\right],$$

and similarly for the regular case,

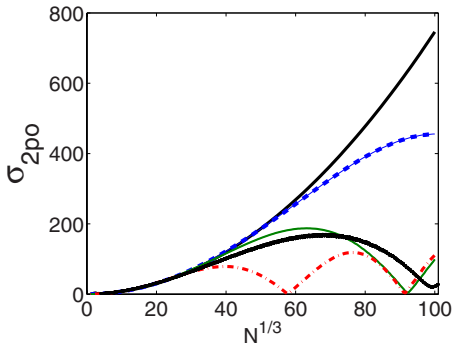

FIG. 1. (Color online) Energy fluctuations $\sigma_{2\text{po}}$ versus particle number $N^{1/3}$ for the HO confinement potential with the two-body interaction strength $g = 0, 0.1, 0.2, 0.4$ (black solid, blue dashed, green thin solid, and red dashed-dotted lines). A corresponding Hartree-Fock result for $g = 0.2$ is shown by the thick solid black line.

$$\sigma_{\text{reg}}^2 = \frac{\hbar^2\tau_H}{6\pi^2\tau_{\min}}\left(\frac{1}{\tau_{\min}^2} - \frac{1}{\tau_T^2}\right).$$

When the trapping potential is harmonic, $V_{\text{trap}} = m\omega^2 r^2/2$ (m is the atom mass; we shall apply $m = 1$), the rather weak two-body interaction between atoms implies that the effective potential Eq. (3) can be approximated by $\omega_{\text{eff}} r^2/2 + \epsilon r^4/4$ [12], implying regular dynamics. Only few periodic orbits appear, and the expression Eq. (9), describing a generic regular system, does not apply. Instead, fluctuations in energy are well described by two periodic orbits, namely, the circular and diameter periodic orbits [12]. The interference of the two orbits gives rise to supershell structure, as noticed in [7]. The semiclassical expression of the energy in terms of these two periodic orbits reproduces very well the result obtained from a microscopic Hartree-Fock calculation.

The second moment of the energy is found by squaring Eq. (4), including only the two shortest periodic orbits. Only the diagonal terms and those corresponding to cosines of the action difference contribute, since the others are eliminated through the averaging procedure due to the rapid fluctuations in the arguments. The resulting expression for the energy variance becomes

$$\sigma_{2\text{po}}^2 = \langle \tilde{U}_{2\text{po}}^2 \rangle \approx 2\hbar^4 \sum_{k=1}^{\infty} \frac{\kappa_T^2}{k^4}\left[\frac{A_d^2}{\tau_d^4} + \frac{A_c^2}{\tau_c^4} - \frac{A_d A_c}{\tau_c^2\tau_d^2}\left\langle \cos\left[k\frac{(S_d - S_c)}{\hbar}\right]\right\rangle\right], \tag{11}$$

where A_d and A_c are amplitudes of the diameter and circle orbits, respectively [12]. The temperature dependence simply appears in the prefactor κ_T [Eq. (5)]. The first two terms, corresponding to squares of the two periodic orbits, diverge at the bifurcation point $\epsilon = 0$. Convergence of the expression is, however, restored by the cross term.

In Fig. 1 we show the energy fluctuations $\sigma_{2\text{po}}$ as a function of $N^{1/3}$ for some different interaction strengths $g = 0$ [pure harmonic oscillator (HO)], $g = 0.1$, 0.2, and 0.4. The energy is here (and throughout the paper) expressed in units

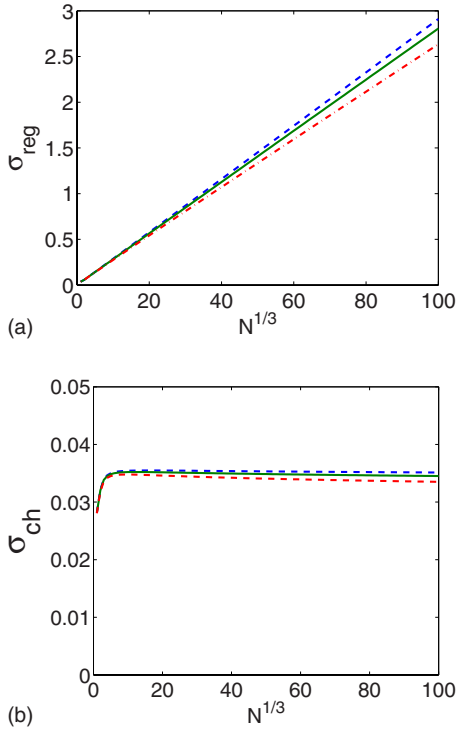

FIG. 2. (Color online) Energy fluctuations versus particle number $N^{1/3}$, assuming a general regular (left-hand figure) or chaotic (right-hand figure) effective potential with the two-body interaction strength $g=0.1,0.2,0.4$ (blue dashed, green solid, and red dashed-dotted lines).

of $\hbar\omega$. Energy fluctuations are seen to decrease with an increasing value of g. Supershell structure implies local minima close to $\sigma_{2\mathrm{po}}=0$. For *larger* values of g the supernode appears at *smaller* particle numbers. In the case $g=0.4$ also the second supernode is seen in Fig. 1. For this interaction strength we also compare to the Hartree-Fock result, which is seen to give a quite similar result.

Energy fluctuations in a generic regular system are described by Eq. (9). Assuming the same scaling with particle number as for the HO for E_C and $\bar{\rho}$ gives energy fluctuations as shown in Fig. 2. No supershell structure appears, but σ_{reg} is found to increase linearly with $N^{1/3}$. The effect of the interaction strength is indeed quite small. Compared to the harmonic confinement potential, Fig. 1, the size of the shell energy fluctuations is notably smaller.

A drastic decrease of energy fluctuations thus appears as the number of contributing periodic orbits increases from one (family) orbit for the pure oscillator ($g=0$ case in Fig. 1) to two dominant orbits for the harmonic confinement with an interacting gas ($g>0$ in Fig. 1), and finally, to the generic regular system [Fig. 2(a); e.g., a potential with steep walls) with several orbits contributing. The diminishing of energy fluctuations with an increasing number of periodic orbits occurs due to destructive interferences from several orbits. The special shell structure with large energy gaps and degeneracies shown by the harmonic oscillator quantum spectrum is less pronounced for systems described by many periodic orbits.

Classical dynamics in the effective potential may become chaotic by properly arranging the confinement potential. In the purely chaotic case the number of periodic orbits increases exponentially with the period time of the orbit and the τ_{min} approximation works well. The fluctuations of the energy originating from chaotic dynamics can thus be calculated by inserting Eq. (8) into Eq. (6). In Fig. 2(b) energy fluctuations for chaotic dynamics is shown versus particle numbers for different values of the interaction strength. For large particle numbers $N>200$, Eq. (10) is a very good approximation of σ_{ch}.

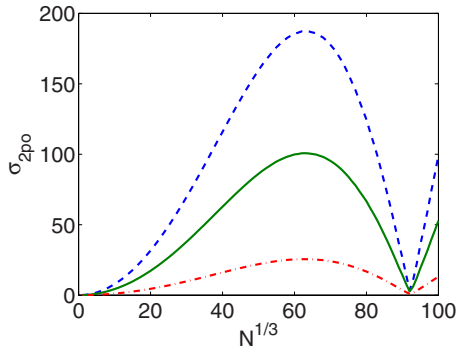

FIG. 3. (Color online) Energy fluctuations versus particle number at different temperatures, assuming a harmonic trapping potential with interaction $g=0.2$. The three curves are valid for temperatures $k_BT/\hbar\omega=0.0,0.1,0.2$ (blue dashed, green solid, and red dashed-dotted lines).

In the case of chaotic dynamics, the energy fluctuations are indeed very small. As compared to the regular case with a harmonic confinement potential, see Fig. 1, the fluctuations are about four orders of magnitude smaller in the chaotic case. The fluctuations are also seen to be fairly independent of particle number and on the interaction strength for $N>100$. The drop in σ_{ch} at smaller particle numbers originates from higher-order terms in the expression for K_{ch} [see Eq. (8)].

Experimental conditions always imply a nonzero temperature, and we shall now investigate the temperature dependence of the energy fluctuations. We assume that the system can be described by the same density of states at $T>0$ as for $T=0$. This implies that the Fermi energy, the periods of the periodic orbits, and the mean level spacing are all assumed independent of temperature. This turns out to be a good approximation for temperatures here studied. The change in temperature thus appears only in the function κ_T, Eq. (5).

The fluctuation in energy at nonzero temperature is obtained by numerically solving Eq. (6) with the form factor given by Eq. (7) for the regular case, and by Eq. (8) for the chaotic case. In the case of a harmonic trapping potential the temperature dependence of the energy fluctuation is directly given by κ_T [see Eq. (11)].

In Fig. 3 the energy fluctuation is shown versus particle number for three different temperatures. For the harmonic trapping potential with $g=0.2$ the supershell structure is clearly preserved but is suppressed with increasing temperature.

The temperature dependence of the energy fluctuations is shown in Fig. 4 for the three studied cases: regular dynamics in a harmonic trap (contribution from two periodic orbits),

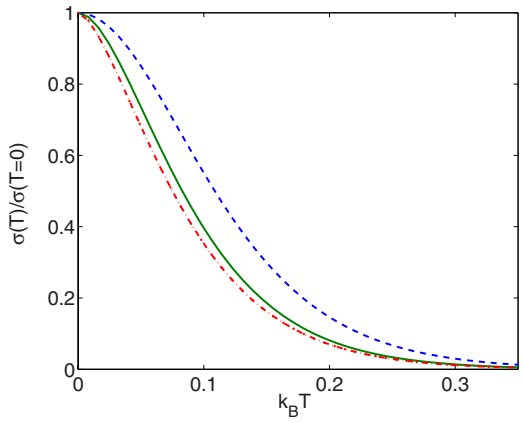

FIG. 4. (Color online) Temperature dependence of energy fluctuation relative to zero temperature for $g=0.2$. HO confinement (blue dashed line), generic regular in $\tau_{\min}$ (green solid line), and chaotic (red dashed-dotted line). Temperature is expressed in units of $\hbar\omega$.

generic regular dynamics, and chaotic dynamics. The fluctuations are shown relative to the $T=0$ fluctuations. All three cases show similar temperature dependence. At a temperature $k_BT \approx 0.1\hbar\omega$ the fluctuations have decreased by 50%, and more or less no energy fluctuations appear for $k_BT > 0.3\hbar\omega$.

In summary, effects from regular and chaotic dynamics have been studied for a trapped dilute gas of interacting fermionic atoms. The fluctuation of the total energy was studied using periodic orbit theory, and three different dynamical systems were considered: regular dynamics in a harmonic trap, general regular dynamics, and chaotic dynamics.

In the case of a harmonic trapping potential a very small number of periodic orbits are sufficient to describe the fluctuating part of the energy. If the atoms are not interacting the Hamiltonian has SU(3) symmetry (pure harmonic oscillator), and one (family) orbit appears. This gives rise to a monotonic increase of energy fluctuations with particle number. A weak repulsive interaction between the atoms implies the contribution of two dominating periodic orbits. The two orbits interfere and give rise to supershell structure, where the detailed behavior depends on the interaction strength g. In general, the fluctuations were found to decrease with interaction strength g, and to increase nonmonotonically with particle number.

For a general regular system as, for example, an effective potential with a flat bottom and steep walls, several periodic orbits contribute. The fluctuations of the energy were then found to be proportional to $N^{1/3}$, and to be considerably smaller than for the harmonic trapping potential. The fluctuations are not sensitive to the interaction strength.

If the effective potential is arranged in such a way that the dynamics is chaotic, the energy fluctuations are found to be considerably diminished as compared to the case of regular dynamics. Compared to the case of a harmonic trap, the fluctuations for chaotic dynamics were found to be almost four orders of magnitude smaller for particle numbers $N > 10^4$. This means that the energy fluctuations more or less vanish for the chaotic effective potential, independent of interaction strength and particle number.

Finally, effects of temperature were described in periodic orbit theory. As expected, a nonzero temperature diminishes the energy fluctuations. Similar dependence on temperature was found for the studied different dynamical situations, and the energy fluctuation was found to be 50% smaller at temperature $k_BT \approx 0.1$ in units of $\hbar\omega$, as compared to zero temperature. For a trap frequency of 10^4 s^{-1} temperatures of the order of 10 nK or smaller are thus required to observe significant fluctuations and supershell structure.

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