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Chaos and Interacting Electrons in Ballistic Quantum Dots

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We show that the classical dynamics of independent particles can determine the quantum properties of interacting electrons in the ballistic regime. This connection is established using diagrammatic perturbation theory and semiclassical finite-temperature Green functions. Specifically, the orbital magnetism is greatly enhanced by the combined effects of interactions and finite size. The presence of families of periodic orbits in regular systems makes their susceptibility parametrically larger than that of chaotic systems, a difference which emerges from correlation terms. [S0031-9007(97)05133-8]

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The connection between classical dynamics and wave interference has recently attracted attention in many fields of physics [1], including atomic, mesoscopic, and optical physics. A central question is to what extent the quantum properties of classically regular and chaotic systems differ. On the whole, this question has been addressed for noninteracting systems. It is now known that many quantum properties are, in fact, strongly influenced by the nature of the classical dynamics—the density of states, the quantum corrections to the conductance, and the optical absorption, to name a few.

We wish to address this question for *interacting* systems and, in particular, to investigate the role of the classical dynamics of the noninteracting system in this context. If the interactions are strong, the noninteracting classical dynamics will be of little relevance. However, if the interactions are short range and not too strong, the noninteracting classical dynamics may be important, and its role can be assessed with perturbation theory. This regime is physically relevant: It applies to a high-density two-dimensional electron gas in which the quasiparticles interact weakly through the short-range screened Coulomb interaction. We find that at *first* order in the interaction there is a difference between regular and chaotic systems, but one which is only numerical, not qualitative. Intrigu-

ingly, as the perturbation theory is carried out to *higher* orders a qualitative difference emerges: Thermodynamic properties scale differently with Fermi energy for chaotic and regular systems. This correlation effect shows that the nature of the classical dynamics can have a substantial effect on the quantum properties of an interacting system.

To be specific, we study the magnetic response of an ensemble of ballistic quantum dots formed from a two-dimensional electron gas. Recent fabrication progress has made possible phase-coherent electronic microstructures much smaller than the mean free path. In these “ballistic” quantum dots, one can think of electrons moving along straight lines between specular reflections off the confining potential. Because this motion is qualitatively different from that taking place in bulk materials, a variety of new behavior has been observed [2]. In particular, the magnetic susceptibility of an ensemble of ballistic squares has been measured [3], and a large enhancement over the Landau response was found. First attempts to understand this experiment within noninteracting models pointed to the importance of the classical dynamics [3–5]. The inclusion of interactions in such systems is our main concern, though much of the discussion applies to ballistic structures in general.

For the magnetic response, the high-density expansion [random-phase approximation] of the thermodynamic potential [6] has to be extended by including Cooper-like correlations, as carried out previously for disordered metals [7–9]. Such expansions are typically used beyond the high-density limit and yield reliable results for the bulk provided some sets of terms are properly resummed. We continue to follow this point of view for quantum dots, where the “small parameter” $r_s = r_0/a_0$ is about 2. (πr_0^2 is the average area per electron, and a_0 is the Bohr radius in the material.) We show that these expansions are particularly insightful when combined with a semiclassical approximation from which the connection to the nature of the classical dynamics can be made. Thus, we will assume that $k_F a \gg 1$ (a is the size of the microstructures and k_F the Fermi wave vector) and that the magnetic field B is classically weak (cyclotron radius $\gg a$).

Semiclassical approach.—The perturbation expansion [6,8,9] for the interaction contribution to the thermodynamic potential Ω yields the magnetic susceptibility through $\chi \equiv (-1/a^2)\partial^2\Omega/\partial B^2$. A series of terms is shown in Fig. 1. The screened Coulomb interaction (wavy lines) is treated as local [10], $U(\mathbf{r} - \mathbf{r}') = \lambda_0 N(0)^{-1} \delta(\mathbf{r} - \mathbf{r}')$, with $N(0)$ the density of states and $\lambda_0 = 1$ identifying the order of perturbation. Straight lines represent the “free” finite-temperature Green function in the presence of the confining potential,

$$\mathcal{G}_{\mathbf{r},\mathbf{r}'}(\epsilon_n) = \theta(\epsilon_n) G_{\mathbf{r},\mathbf{r}'}^R(E_F + i\epsilon_n) + \theta(-\epsilon_n) G_{\mathbf{r},\mathbf{r}'}^A(E_F + i\epsilon_n).$$

Here, E_F is the Fermi energy, $\epsilon_n = (2n + 1)\pi/\beta$ are the Matsubara frequencies, and $G^{R,A}$ is the retarded, advanced Green functions related by $G_{\mathbf{r},\mathbf{r}'}^A(E) = [G_{\mathbf{r},\mathbf{r}'}^R(E^*)]^*$.

Semiclassically, G^R is the sum of the contributions $G_{\mathbf{r},\mathbf{r}'}^{R;j}$ of each classical trajectory j from \mathbf{r} to \mathbf{r}' [1]: In 2D,

$$G_{\mathbf{r},\mathbf{r}'}^R(E) \approx \sum_{j:\mathbf{r}\rightarrow\mathbf{r}'} D_j e^{iS_j/\hbar - i\pi\nu_j/2}, \quad (1)$$

where $S_j = \int_{\mathbf{r}}^{\mathbf{r}'} \mathbf{p} \cdot d\mathbf{r}$ is the classical action of trajectory j , $D_j^2 = (\dot{x}\dot{x}')^{-1} |\partial^2 S_j / \partial y \partial y'| / 2\pi(i\hbar)^3$ is the classical density, and ν_j is a Maslov index. Using $(\partial S_j / \partial E) = t_j$ and $(\partial S_j / \partial B) = (e/c)A_j$, where t_j and A_j are the traversal time and area, one finds

$$G_{\mathbf{r},\mathbf{r}'}^{R;j}(E_F + i\epsilon_n, B) = G_{\mathbf{r},\mathbf{r}'}^{R;j}(E_F, B = 0) \times \exp[-\epsilon_n t_j / \hbar] \times \exp[i2\pi B A_j / \phi_0], \quad (2)$$

where $\phi_0 = hc/e$ is the flux quantum. Note that temperature introduces time and length scales $t_T = L_T/v_F = \hbar\beta/\pi$ which exponentially suppress the contributions of

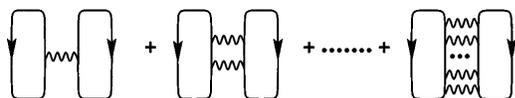


FIG. 1. Leading Cooper-channel diagrams for the interaction contribution to the thermodynamic potential.

long paths through the term $\epsilon_n t_j / \hbar = (2n + 1)t_j / t_T$. (v_F is the Fermi velocity of a billiard.) This provides a complete description in the semiclassical perturbative regime.

We start with the first-order (Hartree-Fock) term in the diagrammatic expansion

$$\Omega^{(1)} = \frac{\lambda_0}{\beta} \sum_{\omega_m} \text{Tr}\{\Sigma_{\mathbf{r},\mathbf{r}'}(\omega_m)\}, \quad (3)$$

where the trace implies an integral over the spatial arguments of the particle-particle propagator [6]

$$\Sigma_{\mathbf{r},\mathbf{r}'}(\omega) = \frac{1}{\beta N(0)} \sum_{\epsilon_n}^{E_F} \mathcal{G}_{\mathbf{r},\mathbf{r}'}(\epsilon_n) \mathcal{G}_{\mathbf{r},\mathbf{r}'}(\omega - \epsilon_n) \quad (4)$$

and $\omega_m \equiv 2m\pi/\beta$. The short-length (high-frequency) behavior is incorporated in the screened interaction, thus requiring a cutoff of the frequency sums at E_F [8]. Semiclassically, $\Sigma_{\mathbf{r},\mathbf{r}'}$ is a sum over pairs of trajectories joining \mathbf{r} to \mathbf{r}' . However, most pairs yield highly oscillating contributions which, after the spatial integrations, give higher-order terms in $1/k_F a$. To leading order, only those pairs contribute to the susceptibility whose dynamical phases $\exp[iS_j(B = 0)/\hbar]$ cancel while retaining a magnetic-field dependence. One way this can be achieved is by pairing each orbit j with its time reverse. The trace in Eq. (3) yields a sum over closed but not necessarily periodic trajectories [see Fig. 2 (left) for a square]. This “diagonal” or “Cooper channel” is present, independent of the nature of the classical dynamics, and we will return to it below. We first turn to an additional contribution present for integrable systems which is central to this paper.

Nondiagonal channel.—In integrable systems, periodic orbits come in families within which the action integral is constant. If, as is generally the case, two orbits of the same family cross at a given point, it is possible to cancel the dynamical phases by pairing them [Fig. 2 (right)]. This pair contributes to the trace in Eq. (3) because both orbits are continuously deformable so that the phase is canceled throughout an entire region of space. For closed but nonperiodic orbits, this condition is met only if they are time reversed (i.e., in the Cooper channel).

This nondiagonal first-order contribution involves a term for each family of periodic orbits. For the square billiard at not too low T ($L_T \lesssim 2a$), only the shortest of

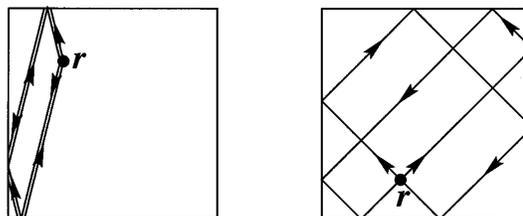


FIG. 2. Typical pairs of real-space trajectories that contribute to the average susceptibility to first order in the interaction in the diagonal channel (left) and the nondiagonal channel (right).

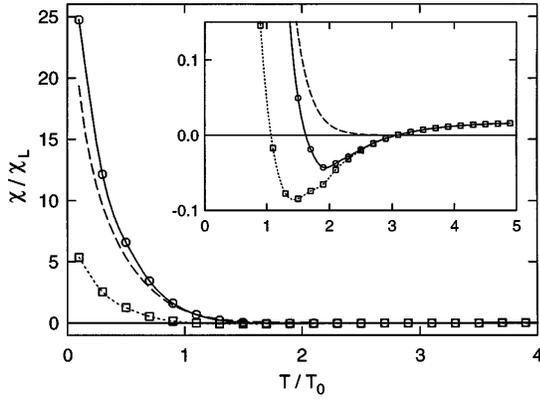


FIG. 3. Temperature dependence of the zero-field susceptibility (solid line) for an ensemble of squares at $k_F a = 50$. The contribution of the nondiagonal channel [dashed, family (11) and repetitions] exceeds that of the diagonal Cooper channel (dotted) at low temperatures ($k_B T_0 = \hbar v_F / 2\pi a$). Inset: expanded scale shows change in sign as a function of T .

these periodic orbits contributes, namely, the family (11) with length $L_{11} = 2\sqrt{2}a$ shown in Fig. 2 (right). In this case, we find for the susceptibility in terms of the Landau susceptibility $\chi_L (= e^2/12mc^2)$

$$\frac{\langle \chi_{11}^{\text{nondiag}} \rangle}{\chi_L} = -\lambda_0 \frac{3k_F a}{4\sqrt{2}\pi^3} \frac{d^2 C^2(\varphi)}{d\varphi^2} R^2 \left(\frac{L_{11}}{L_T} \right), \quad (5)$$

where, as above, one should take $\lambda_0 \equiv 1$ so that the interaction strength is $\bar{U} = N(0)^{-1}$ [10]. The temperature dependence is governed by the function $R(x) = x/\sinh(x)$ and the field dependence by $C(\varphi) = (2\varphi)^{-1/2}[\cos(\pi\varphi)C(\sqrt{\pi\varphi}) + \sin(\pi\varphi)S(\sqrt{\pi\varphi})]$, with $\varphi = Ba^2/\phi_0$ and C and S Fresnel functions. As in the noninteracting case [4,5], the contribution of Eq. (5) is linear in $k_F a$ and has a temperature scale related to the length of the periodic orbit. Quantitatively, the nondiagonal contribution of the family (11) and its repetitions is shown as the dashed curve in Fig. 3. *Thus the existence of a family of periodic orbits—a characteristic of the noninteracting classical dynamics—is associated with an additional first-order interaction contribution to the susceptibility.*

Higher-order terms in perturbation theory also contain nondiagonal contributions. However, in these terms the location of the additional interaction points is severely limited: They must lie on both periodic orbits to cancel the dynamical phases and so must be near the intersections of the two orbits. Further analysis shows that these contributions are therefore smaller by a factor of $1/k_F a$. By contrast, we will now show that the diagonal contribution is strongly renormalized by higher-order terms.

Diagonal Cooper channel.—The first-order contribution to χ in the diagonal channel has the same dependence on $k_F a$ as in Eq. (5) and a similar T dependence; its magnitude is ~ 1.4 times larger. So, to first order in the interaction, the difference between generic chaotic systems—for which there is only the diagonal contribu-

tion—and regular ones—for which the nondiagonal term is also present—is numerical but not qualitative.

However, higher-order diagrams are essential in the diagonal Cooper channel, as known from the theory of superconductivity [6,7]. One should sum all terms which (i) do not vanish upon ensemble averaging, (ii) depend on B , and (iii) are of leading order in $\hbar \sim 1/k_F a$. This yields the Cooper series [6–8] shown in Fig. 1. For instance, (iii) is checked by \hbar power counting, since a pair of Green functions scales as $N(0)/\hbar$, interactions as $[N(0)]^{-1}$, and Matsubara sums as \hbar . Indeed, all terms in the series are of order \hbar despite the formal expansion in λ_0 . Summing the series yields, for the diagonal contribution [8],

$$\Omega^{(D)} = \frac{1}{\beta} \sum_{\omega_m} \text{Tr} \{ \ln [1 + \lambda_0 \Sigma_{\mathbf{r},\mathbf{r}'}^{(D)}(\omega_m)] \}. \quad (6)$$

The diagonal part $\Sigma^{(D)}$ of Σ is a sum over all trajectories longer than the cutoff $\Lambda_0 = \lambda_F/\pi$ [associated with the upper bound E_F on the Matsubara sum in Eq. (4)]:

$$\Sigma_{\mathbf{r},\mathbf{r}'}^{(D)}(\omega_m) \simeq \frac{\hbar}{2\pi N(0)} \sum_{j:\mathbf{r}\rightarrow\mathbf{r}'}^{L_j > \Lambda_0} |D_j|^2 \frac{R(2t_j/t_T)}{t_j} \times \exp[i4\pi B A_j/\phi_0] \times \exp[-\omega_m t_j/\hbar]. \quad (7)$$

While we cannot diagonalize $\Sigma_{\mathbf{r},\mathbf{r}'}^{(D)}$ analytically, it has the nice property that (except for Λ_0) all variations occur on classical scales: Rapid quantum oscillations on the scale of λ_F have been washed out, greatly simplifying the original quantum problem. In this sense, $\Sigma^{(D)}$ is a “classical” operator. Hence, we can discretize $\Sigma^{(D)}$ with a mesh size larger than λ_F , sum over trajectories between cells, and so compute $\Omega^{(D)}$ numerically.

We have performed this computation for the square billiard, obtaining the dotted curve in Fig. 3 for $\chi(T)$. In this curve, we can distinguish three regimes. At low temperature, $\chi^{(D)}$ is *paramagnetic* and decays on a scale similar to the nondiagonal contribution (dashed curve), but has a significantly smaller amplitude. In the intermediate range, $\chi^{(D)}$ is small and *diamagnetic*. Finally, at high temperatures, $\chi^{(D)}$ is again *paramagnetic*, but very small. This is naturally understood by associating each regime with an order in the perturbation series. The low- T part corresponds to the first-order term [orbits of the type in Fig. 2 (left)] which is exponentially suppressed by the temperature factor R when L_T becomes smaller than the shortest closed orbit. At this point the second-order term, due to the closed paths of two trajectories connected by interactions, takes over. There is no minimum length of these paths, and hence the second-order term is less rapidly suppressed by T . For repulsive interactions, the sign is opposite to the first-order term, thus the sign change in $\chi^{(D)}$. At even higher temperatures once $L_T \ll a$, this term is a surface contribution and the third-order term takes over. The latter is a bulk contribution [7] since, with three interactions, flux can be enclosed without bouncing off the boundary.

Renormalization scheme.—This interpretation of Fig. 3 should be reconsidered for two reasons. First, the final result for the diagonal channel at low T is much smaller than the first-order diagonal contribution noted above. Second, one observes numerically that the terms in the perturbation series increase in magnitude with order: One is not in the radius of convergence of perturbation theory but in its analytical continuation. Despite these facts, we show that the interpretation is valid once the interaction entering the diagonal contribution is replaced by a renormalized interaction.

To demonstrate this, we introduce a simple renormalization scheme where integration over short trajectories of length between Λ_0 and a new cutoff Λ yields a decreased effective coupling constant. The new cutoff Λ is larger than Λ_0 but much smaller than any other characteristic length (a , L_T , or $\sqrt{\phi_0/B}$). For each path j joining \mathbf{r} to \mathbf{r}' with $L_j > \Lambda$, let $\Sigma_{\mathbf{r},\mathbf{r}'}^j$ denote its contribution to $\Sigma_{\mathbf{r},\mathbf{r}'}^{(D)}$ and define

$$\begin{aligned} \tilde{\Sigma}_{\mathbf{r},\mathbf{r}'}^j &\equiv \Sigma_{\mathbf{r},\mathbf{r}'}^j - \lambda_0 \int d\mathbf{r}_1 \Sigma_{\mathbf{r},\mathbf{r}_1}^j \hat{\Sigma}_{\mathbf{r}_1,\mathbf{r}'} \\ &+ \lambda_0^2 \int d\mathbf{r}_1 d\mathbf{r}_2 \Sigma_{\mathbf{r},\mathbf{r}_1}^j \hat{\Sigma}_{\mathbf{r}_1,\mathbf{r}_2} \hat{\Sigma}_{\mathbf{r}_2,\mathbf{r}'} + \dots, \end{aligned} \quad (8)$$

where the \mathbf{r}_i integration is over $\Lambda_0 < |\mathbf{r}_{i-1} - \mathbf{r}_i| < \Lambda$ (with $\mathbf{r}_0 \equiv \mathbf{r}$). $\hat{\Sigma}_{\mathbf{r}_1,\mathbf{r}'}$ is defined by Eq. (7) but with the sum restricted to “short” trajectories with lengths in the range $[\Lambda_0, \Lambda]$; $\Sigma_{\mathbf{r},\mathbf{r}_1}^j$ is obtained from $\Sigma_{\mathbf{r},\mathbf{r}'}^j$ by continuously deforming trajectory j . To avoid the awkward \ln in Eq. (6), we introduce $\Gamma = (1/\beta) \sum_{\omega_m} \text{Tr}[1 + \lambda_0 \Sigma_{\mathbf{r},\mathbf{r}'}^{(D)}(\omega_m)]^{-1}$, from which $\Omega^{(D)}$ can be derived through

$$\Omega^{(D)}(\lambda_0) = \int_0^{\lambda_0} \frac{d\lambda'_0}{\lambda'_0} \Gamma(\lambda'_0). \quad (9)$$

Replacing Σ by $\tilde{\Sigma}$ in Γ amounts to a reordering of the perturbation expansion of Γ in which short paths are gathered into lower-order terms. Moreover, if $L_j \gg \Lambda$, small variations in the spatial arguments do not modify noticeably the characteristics of Σ^j . Approximating $\Sigma_{\mathbf{r},\mathbf{r}_1}^j$ by $\Sigma_{\mathbf{r},\mathbf{r}'}^j$ in Eq. (8) and using $\hat{\Sigma}_{\mathbf{r}_1,\mathbf{r}'} \approx 1/4\pi|\mathbf{r}_1 - \mathbf{r}'|^2$ valid for short paths, we obtain

$$\lambda_0 \tilde{\Sigma}_{\mathbf{r},\mathbf{r}'}^j \approx \frac{\lambda_0 \Sigma_{\mathbf{r},\mathbf{r}'}^j}{1 + \lambda_0 \int d\mathbf{r}_1 \hat{\Sigma}_{\mathbf{r}_1,\mathbf{r}'}} \approx \lambda(\Lambda) \Sigma_{\mathbf{r},\mathbf{r}'}^j, \quad (10)$$

where the running coupling constant is defined by $\lambda(\Lambda) = \lambda_0/[1 + (\lambda_0/2) \ln(\Lambda/\Lambda_0)]$. Therefore, these steps amount to a change of both the coupling constant and the cutoff (since now trajectories shorter than Λ must be excluded) without changing Γ ; that is, $\Gamma(\Lambda_0, \lambda_0) = \Gamma(\Lambda, \lambda(\Lambda))$. Through Eq. (9), this renormalization scheme can be applied to $\Omega^{(D)}$, and so to the average susceptibility.

In this way, we have eliminated the last “quantum scale” Λ_0 from $\Sigma^{(D)}$: Λ can be made much larger than λ_F while

remaining smaller than all classical lengths. Furthermore, it is qualitatively reasonable that the perturbation series of $\Omega^{(D)}$ becomes convergent when Λ is of order a , since by this point the spread in length scales causing the divergence has been eliminated. We have checked that this is true numerically, although this is at the border of the range for a quantitative answer. The conclusion from this renormalization argument is that $\lambda(a) \approx 2/[2 + \ln(k_F a)]$ replaces the coupling constant $\lambda_0 = 1$ in the perturbative expressions for the diagonal channel.

Consequently, for large k_F at low T ($L_T \geq$ shortest periodic orbit), the diagonal contribution is *parametrically* smaller than the nondiagonal contribution by a factor $1/\ln(k_F a)$ because higher-order correlation terms reduce only the diagonal contribution. *Therefore, regular systems, for which there is a nondiagonal contribution, show a magnetic response logarithmically larger than the generic chaotic systems, for which only the diagonal channel is open.* For comparison, we note that the non-interacting contribution obtained previously [4,5] is of the same order as this interaction contribution for integrable systems but smaller for chaotic ones.

The reduction factor provided by $\lambda(a)$ allows one to understand qualitatively, first, why the diagonal contribution is less than the off-diagonal one in Fig. 3 and, second, why the diamagnetic excursion and high-temperature tail are small. Thus, the interpretation above of the diagonal channel is correct once $\lambda(a)$ replaces λ_0 .

With the nondiagonal channel, the magnitude of χ that we find is in good agreement with the experiment at the lowest experimental temperatures [3]. However, the temperature scale T_0 in Fig. 3 is significantly smaller than that in the experiment: After an initial rapid decay, the experimental susceptibility decreases slowly as T increases. The reason for this slow decay is not known.

In conclusion, we have shown that a semiclassical treatment allows one to study the high-density perturbative expansion of the interaction contribution to the grand potential for ballistic quantum dots. This semiclassical approach is an efficient tool to compute quantitatively the magnetic response. Moreover, when combined with a renormalization scheme, it provides an intuitive picture of various features specific to the ballistic regime. The most striking one is that the susceptibilities of integrable and chaotic geometries scale differently with $k_F a$ because of the presence of families of periodic orbits in the former. Another unusual property, caused by the different T dependence of different orders in the (renormalized) interaction, is that with increasing temperature the interaction contribution changes sign from paramagnetic to diamagnetic and then back to paramagnetic.

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- [10] This amounts to neglecting the momentum dependence of the Thomas-Fermi potential, which in two dimensions is $\hat{U}(p) = N(0)^{-1}/[1 + r_s^{-1}\sqrt{1/2}(p/p_F)]$. Since the momentum transfers along the trajectories we consider are of order p_F , we may replace $\hat{U}(p)$ by $\hat{U}(0)$ for typical r_s .