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Quantum oscillations in confined and degenerate Fermi gases. II. The phase diagram and applications of half-vicinity model

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ABSTRACT

For part I see DOI: 10.1016/j.physleta.2018.02.006. Size and density dependent quantum oscillations appear in Fermi gases under strong confinement and degeneracy conditions. We provide a universal recipe that explicitly separates oscillatory regime from non-oscillatory (stationary) one. A phase diagram representing stationary and oscillatory regimes on degeneracy-confinement space is proposed. Analytical expressions of phase transition interfaces are derived. The critical point, which separates entirely stationary and oscillatory regions, is determined and its dependencies on aspect ratios are examined for anisometric domains. Accuracy of the half-vicinity model and the phase diagram are verified through the quantum oscillations in electronic heat capacity and its ratio to entropy.
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1. Introduction

This article constitutes the second part of a two-part article. In the first part of this paper [1], to which we shall refer as “Article I” hereafter, we have built an analytical model called half-vicinity model (HVM) for the prediction and accurate calculation of size and density dependent oscillations in thermodynamic and transport properties of confined and degenerate Fermi gases. Analytical construction, derivations and detailed examination of HVM can be found in Article I (Ref. [1]).

In this part, we construct a phase diagram for quantum oscillations. The phase diagram is established on HVM and considers half-vicinity (HV) states, off-half-vicinity (OHV) states and the balance conditions between them. Although different types of phase diagrams have been proposed under quantum oscillation regime in literature [2–4], a phase diagram separating oscillatory and stationary regimes has never been proposed for any dispersion relation.

The proposed phase diagram for systems having quadratic dispersion relation is used to predict size and density dependent quantum oscillations in Fermi systems. Moreover, it can easily be modified for systems having linear ones also [5–33].

In the following section of this paper, a phase diagram of quantum oscillations is established and phase transition interfaces between stationary (classical, continuous) and oscillatory (quantum, discrete) regimes are analytically given for 1D, 2D and 3D cases. Critical confinement and degeneracy values, which separates entirely stationary and oscillatory regions, are also determined by considering their aspect ratio dependencies. In Sec. 3, results of exact (definitional expressions based on infinite sums) and HVMs are compared for size and density dependent oscillations in the electronic specific heat capacity of strongly degenerate and confined ideal Fermi gases. Finally, broken equivalence of entropy–heat capacity in quantum degenerate limit of ideal Fermi gases is also well predicted by HVM.

2. A phase diagram for quantum oscillations: transition from classical to quantum behavior

Occupancy variance function is given in Article I as

$$\sigma^2(i_1,\ldots,i_d)=\frac{\partial f}{\partial\Lambda}=-\frac{\partial f}{\partial\tilde{\varepsilon}}=\frac{g_s}{4}\,\mathrm{sech}^2\left(\frac{\tilde{\varepsilon}-\Lambda}{2}\right), \quad (1)$$

where $f=g_s/[\exp(-\Lambda+\tilde{\varepsilon})+1]$ is Fermi–Dirac distribution function, g_s is spin factor, $\Lambda=\mu/(k_BT)$ is dimensionless chemical potential and dimensionless energy eigenvalues are denoted as $\tilde{\varepsilon}=\varepsilon/(k_BT)=(\alpha_1 i_1)^2+\cdots+(\alpha_d i_d)^2$ for a d-dimensional rectangular confinement domain, where i_n is quantum state variable for a particular direction $n=\{1,2,\cdots,d\}$. The confinement parameter is written as $\alpha_n=h/\left(\sqrt{8mk_BT}L_n\right)$.

Total occupancy variance (TOV) in its exact summation form is written as

$$\Sigma_D^2=\sum_{i_1=1}^{\infty}\cdots\sum_{i_d=1}^{\infty}\sigma^2(i_1,\ldots,i_d). \quad (2)$$

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This function can be approximated in continuum and degenerate limit as

$$\Sigma_{CA}^2 = \frac{g_s \pi^{d/2}}{2^d \alpha_1 \cdots \alpha_d} \frac{\Lambda^{(d-2)/2}}{\Gamma(d/2)}. \tag{3}$$

Two equations below are from the Article I where the methodology of HVM is constructed. In HVM, TOV is derived as

$$\Sigma_{HV}^2 = \sum_{i_1=1}^{\infty} \cdots \sum_{i_d=1}^{\infty} \sigma^2 w_{HV}. \tag{4}$$

In continuum limit, it is approximated by

$$\Sigma_{HVC}^2 \cong \tanh\left(\frac{\delta_{\tilde{\varepsilon}}}{4}\right) \Sigma_{CA}^2, \tag{5}$$

where $\delta_{\tilde{\varepsilon}}$ is the thickness of half-vicinity shell in dimensionless energy space (for its expressions see Eqs. (10a), (11) and Table I from Article I).

HVM takes the discreteness of quantum states into account and allows us to accurately calculate thermodynamic and transport properties exhibiting size and density dependent quantum oscillations without using infinite summations. In addition to that, HVM can accurately estimate where the transition from classical behavior to quantum behavior starts, in the framework of quantum oscillations.

The states contributing to TOV consist of HV states and OHV states (*i.e.*, $\Sigma_D^2 = \Sigma_{HV}^2 + \Sigma_{OHV}^2$). HV states are responsible from the oscillatory part of TOV, whereas OHV states represent the stationary part, see Article I. They constitute two competing parts of TOV. Domination of contributions of HV states over OHV ones leads to oscillations and vice versa. Hence, by considering $\Sigma_{HV}^2 = \Sigma_{OHV}^2$ balance, we can compare contributions of HV states and OHV states to define a universal (material independent) recipe for the separation of stationary regime (SR) from oscillatory regime (OR). According to the recipe, when $\Sigma_{HV}^2 < \Sigma_{OHV}^2$, oscillations disappear (SR) and on the opposite condition $\Sigma_{HV}^2 > \Sigma_{OHV}^2$, oscillations reveal (OR). Since $\Sigma_{OHV}^2 = \Sigma_D^2 - \Sigma_{HV}^2$, SR–OR transition can be quantified as the balance of the contributions of HV and OHV states ($\Sigma_{HV} = \Sigma_{OHV}$) by $\Sigma_D^2 = 2\Sigma_{HV}^2$.

Since the transition is not sharp but smooth, we can safely use analytical expressions of TOV, instead of their exact expressions, to find an analytical expression for SR–OR separation. From the balance condition between contributions of HV and OHV states as well as Eq. (5), we can determine the following analytical condition for the transition between SR and OR,

$$\Sigma_{CA}^2 = 2\Sigma_{HVC}^2 \Rightarrow 1 = 2\tanh(\delta_{\tilde{\varepsilon}}/4) \Rightarrow \delta_{\tilde{\varepsilon}} = 2\ln 3. \tag{6}$$

As is seen from red curve in Fig. 3 in Article I, balance condition quantified in Eq. (6) clearly gives the SR–OR separation. By decreasing confinement or degeneracy, the number of states around Fermi level increases, contributions of OHV states become also appreciable and their contributions make oscillation amplitude smaller. The more number of states around Fermi level, the smaller oscillation amplitude. When contributions of OHV states exceeds that of HV states, oscillations disappear.

To complete the construction of phase diagram, it is necessary to check also the number of particles, (N), inside the system, since we are dealing with extremely confined systems having relatively low number of particles. For statistical representations there has to be sufficiently large number of particles inside the system. Nevertheless, the physically meaningful region in a phase diagram can be stated by the condition $N \geq 1$. Full list of recipes and conditions to establish the phase diagram is given in Table I.

According to the recipes and conditions given in Table I, phase diagrams of quantum oscillations in degeneracy-confinement space for various dimensions can be determined. For isometric 3D domains, the phase diagram is constructed and given in Fig. 1. Solid-black curves represent interfaces defined by the conditions in Table I. $\delta_{\tilde{\varepsilon}} = 2\ln 3$ condition, representing the balance of HV and OHV states, separates OR and SR. As long as degeneracy is sufficiently high, it's possible to control the quantum oscillations in thermodynamic and transport quantities by controlling the confinement parameter.

Table I
Recipes and conditions for the construction of the phase diagram of quantum oscillations.

Region	Recipe	Condition
OR	$\Sigma_{HV}^2 > \Sigma_{OHV}^2$	$\delta_{\tilde{\varepsilon}} > 2\ln 3$
SR	$\Sigma_{HV}^2 < \Sigma_{OHV}^2$	$\delta_{\tilde{\varepsilon}} < 2\ln 3$
Unphysical	$N < 1$	$\sum_{i_1,\ldots,i_d=1}^{\infty} f < 1$

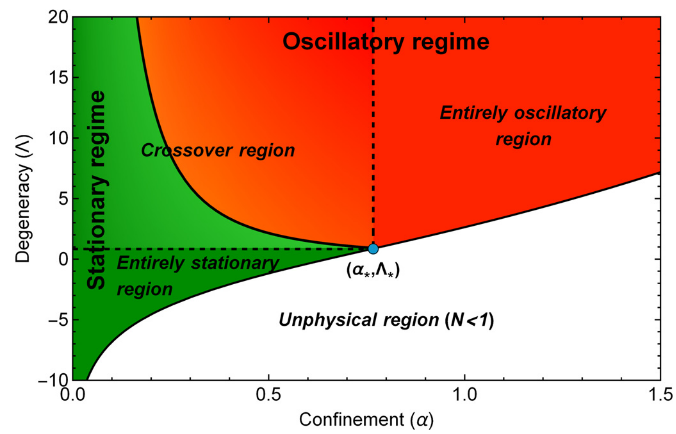

Fig. 1. (Color online.) A phase diagram for quantum oscillations on degeneracy-confinement space in case of isometric 3D confinement domains. $\delta_{\tilde{\varepsilon}} = 2\ln 3$ condition defines the boundary between stationary (classical) and oscillatory (quantum) regimes. Blue dot represents the critical point in the phase diagram.

Table II
Conditions and regions of the phase diagram.

Conditions	Regions
$\alpha < \alpha_*$, $\Lambda < \Lambda_*$, (check $N > 1$)	Entirely SR
$\alpha < \alpha_*$, $\Lambda > \Lambda_*$	Crossover region
$\alpha > \alpha_*$, $\Lambda > \Lambda_*$, (check $N > 1$)	Entirely OR
$\alpha > \alpha_*$, $\Lambda < \Lambda_*$	Unphysical region

Intersection of SR–OR interface curve with $N = 1$ curve denotes the critical point which is represented by blue dot in Fig. 1. Critical value of the confinement parameter at this point is $\alpha_*^{3D} = 0.78$ and the corresponding degeneracy value is $\Lambda_*^{3D} = 0.88$. These values are universal for isometric rectangular confinement domains. For confinement values below α_*, existence of oscillations can be controlled and they can even be suppressed by decreasing degeneracy (through density or temperature). Similarly, for degeneracy values higher than Λ_*, existence of oscillations can be controlled by changing confinement. This region defined by $\{\Lambda > \Lambda_*, \alpha < \alpha_*\}$ is the crossover region restricted by dashed lines in the phase diagram. On the contrary, for higher confinement values than α_*, quantum oscillations cannot be suppressed and the region is called entirely oscillatory region. Below the critical degeneracy values, system does not exhibit oscillatory behaviors regardless of the values of confinements. Hence, this critical point is used to define different regions (crossover region, entirely OR and entirely SR). Regimes on phase diagram and corresponding conditions are summarized in Table II.

Although the phase diagram in Fig. 1 represents only isometric 3D domain, the form of the phase diagrams for 1D and isomet-

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