Low temperature resonances in the fermion heat capacity of finite systems.

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Abstract. Temperature variations of the heat capacity ($C$) are studied in a low temperature regime $T < \varepsilon_F/N$ ($\varepsilon_F$ is the Fermi energy) for 2D- and 3D-systems with $N \sim 10^2 \div 10^4$ treated as a canonical ensemble of $N$-noninteracting fermions. The analysis of $C$ is performed by introducing a function $\varphi(\varepsilon)$, the spectral distribution of $C$ that gives the contribution of each single-particle state to $C$. The function $\varphi(\varepsilon)$ has two peaks divided by the energy interval $\Delta \varepsilon \approx (2 \div 5) T$. If at some temperature $T_{\text{res}}$ there takes place a resonance i.e. the positions of these peaks coincide with energies of two levels nearest to $\varepsilon_F$ then $C$ vs $T$ shows a local maximum i.e. $T_{\text{res}}$ is determined by single-particle level spacings near the Fermi level.

1. Introduction

Among many experiments performed to the present time on mesoscopic systems there are only several investigations of their thermal properties ([1] and references therein) though studying the electron heat capacity ($C$) of normal (nonsuperconducting) mesoscopic systems could give valuable information concerning the electron level structure in the vicinity of the Fermi energy.

In bulk samples the electron heat capacity $C$ linearly increases with $T$

$$C/k_B = \frac{\pi^2}{3} \rho_0(\varepsilon_F) k_B T$$

($\rho_0(\varepsilon_F)$ is the electron state density in the vicinity of $\varepsilon_F$) and this law is fulfilled in a wide low temperature range, $0 \leq T \ll \varepsilon_F$, irrespective of the size and shape of the body. In finite systems Eq. (1) is applicable down to an interval of $T$ of order of $\delta_F$, the mean level spacing near $\varepsilon_F$. Within it $C$ increases exponentially and can display some local extrema.

$$\delta_F = \overline{d_F}/\rho_0(\varepsilon_F) \sim \varepsilon_F/N,$$

($d_F$ is the average level degeneracy near $\varepsilon_F$. As a rule $d_F = 2$ for asymmetric systems and $\overline{d_F} > 2$ for symmetric ones).

We describe this range of the heat capacity variation in the framework of the Noninteracting Particle Model ($NPM$) that idealizes and simplifies the real picture of the electron movement in mesoscopic systems as it neglects effects of disorder, Coulomb and electron - phonon interactions. However we believe that detailed ascertainment of the mean field role can help to reveal the impact of the other factors on measured thermodynamic quantities.
The temperature scale in finite fermion systems explicitly depends on $\varepsilon_F$ that is material dependent and for systems with identical $N$ can differ by orders magnitude. Therefore, not to be bound to an individual mesoscopic system we measure all energies and the temperature in $\delta_F$. Thus all results of our calculations can be projected on any fermion system if its $\varepsilon_F$ is known. We suppose that $\delta_F$ is much less than the Debye temperature otherwise the electron heat capacity cannot be observed.

Independently of the type of electron confinement and of that whether a system is integrable or not the common feature of electron energy spectra in different finite systems consists in the appearance of such irregularities in the eigenvalue distributions as level bunchings or high degenerated levels in systems possessing some symmetry. These irregularities can reveal themselves in measured quantities e.g. in the low temperature electron heat capacity. This fact was for the first time established by Frölich [2] for a model spectrum with high degenerated levels. Later an analogous result was obtained for spherical alkali clusters by Brack et al [4] where the single-particle potential was found by the temperature Hartree-Fock method. In both cases the low temperature variation of the heat capacity displays local maxima at those particle numbers which correspond to completely occupied high degenerated levels. On the other hand the calculations of Denton et al [3] showed that a uniform single-particle spectrum with spin degenerated levels and equal spacings between them practically gives a monotonous increase of the heat capacity, which is particularly appropriate to analyze contributions of single-particle levels nearest to $\varepsilon_F$. The results has stimulated us to look for the cause of such different behavior of $C$ vs $T$.

2. The spectral distribution of the heat capacity and local maxima in $C$

In Ref. [5] we have developed a canonical polynomial method for studying finite systems with a fixed $N$ in $NPM$. Here the method is modified to introduce the spectral distribution of the heat capacity, $\varphi(\varepsilon)$, which is particularly appropriate to analyze contributions of single-particle levels to $C$ and allows us to connect the appearance of the low temperature maxima in $C$ with the level structure near $\varepsilon_F$.

\[ \varphi(\varepsilon) = (\varepsilon - \varepsilon_0) \frac{\partial n(\varepsilon)}{\partial T}, \quad C/k_B = \int_0^\infty \rho(\varepsilon)\varphi(\varepsilon)d\varepsilon, \quad (3) \]

$\rho(\varepsilon) = \sum_i \delta(\varepsilon - \varepsilon_i) d_i$ is the exact state density ($\varepsilon_i, \ d_i \geq 1$ are respectively the energy and degeneracy of the single-particle level $t$). Thus Eq. (3) shows that $\varphi(\varepsilon)$ is the contribution to $C$ of one electron on level $t$; $n(\varepsilon)$ is the canonical distribution of occupation numbers [5], $\varepsilon_0$ is a constant which does not affect the values of $C$. Function $\varphi(\varepsilon)$ can be viewed as an averager of $\rho(\varepsilon)$. In the effective grand canonical approximation $n(\varepsilon)$ is replaced by the Fermi-Dirac function $f(\varepsilon)$ with the temperature dependent chemical potential $\lambda$ providing the particle number conservation at any $T$. Functions $\varphi(\varepsilon)$ and $\varphi_{eff}(\varepsilon) = \varphi(\varepsilon; n(\varepsilon) \rightarrow f(\varepsilon))$ have two peaks divided by a minimum in which both functions are equal to zero if $\varepsilon_0 = \lambda + \beta\partial\lambda/\partial\beta$, ($\beta = 1/T$). The energy distance $\Delta\varepsilon$ between two peaks of $\varphi_{eff}(\varepsilon)$ is always equal $\approx 5T$ while for $\varphi(\varepsilon)$ the distance $\Delta\varepsilon$ is of the order of or less than $5T$ and depends on the level structure.

At some temperature $T_{res}$ the positions of two peaks of $\varphi(\varepsilon)$ coincide with the energies of levels nearest to $\varepsilon_F$, e.g. for systems with even $N$ it can be levels $F$ and $F + 1$ that can cause the appearance of the local maximum in $C$ at

\[ T_{res} = \xi(\varepsilon_{F+1} - \varepsilon_F), \quad \xi \sim 0.2 \div 0.5 \quad (4) \]

if the contribution of other levels to $C$ is significantly less i.e. if at this temperature $\varphi(\varepsilon)$ cuts out from the single-particle spectrum practically only two these levels.

To show how the spectral heat capacity $\varphi(\varepsilon)$ forms the peak in the canonical $C$ we use the equidistant spectrum model with degenerated levels (the level spacing is equal to $\delta$) and
consider systems with even $N$ and completely filled (at $T = 0$) level $F$. Fig. 1a shows that the low temperature peak arises in the model with the high level degeneracy ($d = 10$) as at $T = 0.24\delta$ the positions of two peaks of $\varphi(\varepsilon)$ coincide with energies of levels $F$ and $F + 1$, Fig.1b. Although at $T = 0.3\delta$ for $d = 2$ the positions of two peaks of $\varphi(\varepsilon)$ coincide with energies of levels $F$ and $F + 1$ too, the peak in $C$ is absent because for $d = 2$ the contributions of $(F - 1)$-, and $(F + 2)$-levels to $C$ are comparable with those of $F$-, and $(F + 1)$-levels contrary to the case with $d = 10$ where $F$-, and $(F + 1)$-levels contribute to $C$ several times more than other levels, Fig. 1b. It should be mentioned that at $d \gg 1$ the canonical and effective grand canonical heat capacities practically coincide.

Figure 2. Left panel: The heat capacity (in units of $C_{lin}$) with two resonances for $10^4$ fermions in a briquette cavity. $t_1$ and $t_2$ are the positions of the maxima. $t = T/\delta_F$, $\delta_F = 4\varepsilon_F/3N$. The ratio of briquette lateral lengths $L_x : L_y : L_z = 1 : 0.6e : \pi$ provides only the spin degeneracy of the single-particle levels. Right panel: The spectral heat capacity $\varphi(\varepsilon)$ at these temperatures. The first maximum is practically at $t_1 = (\varepsilon_{F+1} - \varepsilon_F)/5\delta_F$, the second maximum at $t_2$ corresponds to the presence of two level bunches in the vicinity of the peaks in $\varphi(\varepsilon)$. The vertical lines mark the level positions.

However the small level degeneracy does not generally except the local maxima. If near $\varepsilon_F$ a group of doubly degenerated levels is concentrated so that spacings between them are much smaller then the distance from this group to other levels the appearance of local maxima are also possible as it is shown e.g. for a briquette system with $N = 10^4$ in Fig. 2.

Fig. 3 shows that at continuous alteration of some parameter $\alpha$ characterizing deformation
Figure 3. Top panel: Shape oscillations of the low temperature canonical heat capacity of the system with \( N = 42 \) fermions moving in 2D oscillator potential. \( \omega_x, \omega_y \) are the oscillator frequencies. \( \delta_F = \varepsilon_F / 2N \). Bottom panel: Behavior of electron energy levels near the Fermi level (bold line). Solid circles are the crossing points of the Fermi level and upper levels free from electrons at \( T = 0 \).

of a system (\( \alpha = \omega_x / \omega_y \) in the 2D-oscillator case) \( C \) can display oscillations vs \( \alpha \) with minimum values of \( C \) at such deformation where the system gains an additional symmetry.

These examples demonstrate that measuring \( T_{\text{res}} \) can give information concerning the level spacings and distributions of single-particle levels near the Fermi level.

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