Stability of matter p. 6

10. LT and semiclassics

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The semiclassical approximation in quantum mechanics uses the classical concept of a phase space to describe spectral properties of quantum mechanical systems.

Note that the sum of eigenvalues can be written as the trace of negative part of the Schrödinger operator:

$$\sum_{j\geq 0} E_j = \mathrm{Tr}\,(-\Delta + V)_-$$

Tracing over the Hilbert space in QM means testing against all possible states – classically this corresponds to exploring the whole phase space (digression: all this can be made rigorous and precise → quantization course).

So, in the semiclassical approximation we have

$$\mathrm{Tr}\,(-\Delta+V)_- \simeq c \iint_{\mathbb{R}^3\,\mathbb{R}^3} dp\,dx \; \mathbb{1}\left(p^2+V(x)\leq 0\right)$$

The constant c corresponds to the fact that one quantum state has certain volume in the phase space. In fact, the constant c is equal $(2\pi\hbar)^{-3}$, or rather $(2\pi)^{-3}$ in our units (note: in this section we use $-\Delta$ and not $-\frac{1}{2}\Delta$).

Digression: why $(2\pi\hbar)^3$?

consider a box o side length L, volume $V=L^3$

A QM particle wave-function is of the form

$$\psi(x,y,z) \simeq \sin(k_x x)\sin(k_y y)\sin(k_z z)$$

where Dirichlet boundary conditions (vanishing upon the walls) imposes

$$k_i = \frac{n_i \pi}{L} \qquad (k\text{-space cell volume } (\tfrac{\pi}{L})^3)$$

$$\Rightarrow \text{energy} \qquad \varepsilon_k = p^2 = (\hbar k)^2 = n^2 \varepsilon_0$$

with $\varepsilon_0 = \dfrac{\pi^2\hbar^2}{L^2}$, $n^2 = n_x^2 + n_y^2 + n_z^2$.

The states available to a particle in a box can be represented by points on a 3-dim. lattice $\{k_x, k_y, k_z\}$. All distinct states are represented by points with $k_i \geq 0$ (sign of wave-function)

Total number of states in the spherical shell with radius between k and $k+dk$ is then the volume of one octant of a spherical shell divided by the cell volume:

$$d\Gamma = \frac{1}{8}\,\frac{4\pi k^2\,dk}{(\pi/L)^3} = \frac{V}{(2\pi)^2}\,k^2\,dk$$

since $p = \hbar k$ we get

$$d\Gamma = \frac{d^3 r \, d^3 p}{(2\pi\hbar)^3}$$

Digression 2:

the above argument has been demonstrated for a cube, but for large volumes the result is independent of the shape of the domain : Weyl's law !

can one hear the shape of a drum ? (M. Kac)

Ok, so we know

$$\sum_{j\geq 0} |E_j|^0 \approx \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \mathbb{1}(p^2 + V(x) \leq 0) \, dp \, dx$$

and similarly

$$\sum_{j\geq 0} |E_j|^\gamma \cong \frac{1}{(2\pi)^3} \iint_{\mathbb{R}^3 \, \mathbb{R}^3} \mathbb{1}(p^2 + V(x) \leq 0) \, |p^2 + V(x)|^\gamma \, dp \, dx$$

We can calculate :

$$\iint_{p^2+V(x)\leq 0} |p^2 + V(x)|^\gamma = \int_{\mathbb{R}^3} \int_{|p|\leq \sqrt{|V_-|}} (|V_-(x)| - p^2)^\gamma \, dp \, dx$$

$$= \int_{\mathbb{R}^3} |V_-(x)|^{\gamma+\frac{3}{2}} dx \int_{|q|\leq 1} (1-q^2)^\gamma \, dq$$

This last integral can be computed:

$$\int_{|q|\leq 1} (1-q^2)^\gamma \, dq = \frac{\Gamma(\gamma+1)}{(4\pi)^{\frac{d}{2}} \, \Gamma(\gamma+1+\frac{d}{2})} =: L^{cl}_{\gamma,d}$$

The question how the constant in the Lieb-Thirring inequality $L_{\gamma,d}$ is related to the semiclassical constant $L^{cl}_{\gamma,d}$ has become an important problem in spectral theory.

Weyl asymptotics imply that $L^{cl}_{\gamma,d} \leq L_{\gamma,d}$

- Lieb-Thirring (1981): $L^{cl}_{\gamma,d} = L_{\gamma,d}$ for $d=1$, $\gamma \geq \frac{3}{2}$
- Laptev-Weidl (2000): —"— $\gamma \geq \frac{3}{2}$, $d \geq 1$
- also known $L_{\frac{1}{2},1} = 2 L^{cl}_{\frac{1}{2},1} = \frac{1}{2}$
- for $\frac{1}{2} \leq \gamma < \frac{3}{2}$ in $d=1$ and $\gamma < 1$ in $d \geq 1$ it is known that $L^{cl}_{\gamma,d} < L_{\gamma,d}$
- most recent improvement: Frank-Hundertmark-Jex-Nam (2021)

  $d \geq 1$

$$L_{1,d} \leq 1{,}456 \, L^{cl}_{1,d}$$

Related to optimal constants in Gagliardo-Nirenberg and Sobolev inequalities, harmonic analysis...