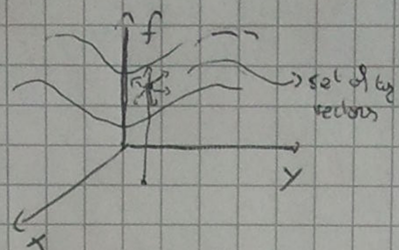
TOPICS IN COND. MATTER. Lecture 2

MATHS: EXTREMA IN PRESENCE OF CONSTRAINTS

$f(x,y)$



A 2D-SURFACE: $(x, y, f(x,y))$
$\forall x, y \in D \subseteq \mathbb{R}^2$.

RECALL: EXTREMA OF $f(x,y)$.

THE EXTREMA OF $f(x,y)$ ARE OBTAINED BY IMPOSING

$$\vec{\nabla} f = (\partial_x f, \partial_y f) = (0,0)$$

NAMELY, FOR A GIVEN POINT $(x_0, y_0, f(x_0,y_0))$ THE SET OF VECTORS TANGENT TO THE SURFACE IS GIVEN BY:

$$\vec{Y} = \left(a, b, a\,\partial_x f\big|_{(x_0,y_0)} + b\,\partial_y f\big|_{(x_0,y_0)}\right)$$

WHERE a, b ARE ARBITRARY NUMBERS.

THE $\vec{Y}_s$ ARE PARALLEL TO THE XY-PLANE (I.E. MAXIMUM, MINIMUM OR SADDLE POINT) IF

$$a\,\partial_x f\big|_{x_0,y_0} + b\,\partial_y f\big|_{x_0,y_0} = 0 \quad \forall a, b \to \partial_x f\big|_{x_0,y_0} = \partial_y f\big|_{x_0,y_0} = 0.$$

REMIND THAT, ONCE YOU DETERMINED THE EXTREMA, YOU CAN DETERMINE ITS NATURE BY STUDYING THE HESSE MATRIX:

$$x_0, y_0 \,/\, (\partial_x f)_{x_0,y_0} = (\partial_y f)_{x_0,y_0} = 0$$

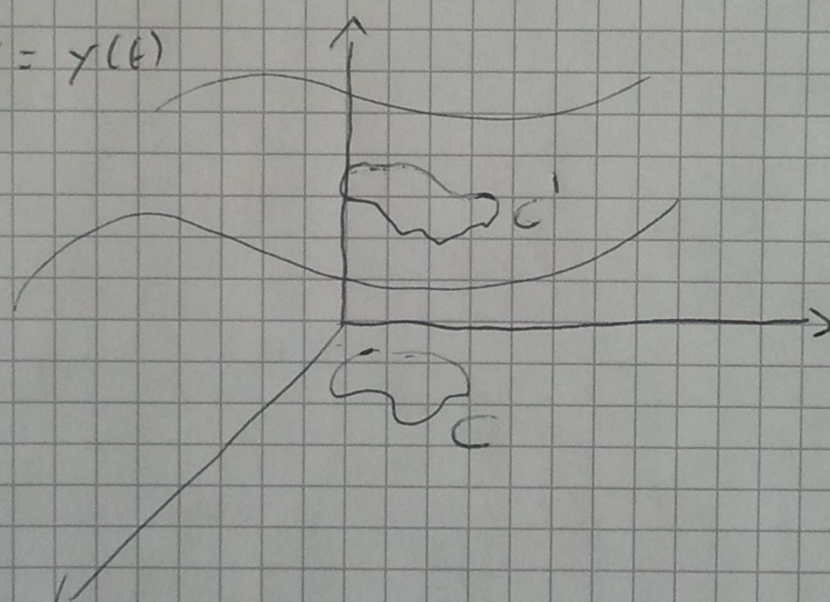
$$H\big|_{x_0,y_0} = \frac{1}{2}\begin{pmatrix} \partial_x^2 f\big|_{x_0,y_0} & \partial_x\partial_y f\big|_{x_0,y_0} \\ \partial_y\partial_x f\big|_{x_0,y_0} & \partial_y^2 f\big|_{x_0,y_0} \end{pmatrix}$$

(NOTE: H IS SYMMETRIC AND REAL)

$$\begin{cases} \text{IF } \lambda_1 > 0, \lambda_2 > 0 \mapsto \text{MINIMUM} & \text{(LOCAL MINIMUM IN GENERAL)} \\ \text{IF } \lambda_1 < 0, \lambda_2 < 0 \mapsto \text{MAXIMUM} & \text{(LOCAL MAXIMUM " ")} \\ \text{IF } \lambda_1 \cdot \lambda_2 < 0 \mapsto \text{SADDLE POINT} & \end{cases}$$

THEN, LET US CONSIDER A CONSTRAINT IN THE DOMAIN $D \subseteq \mathbb{R}$
THIS CONSTRAIN CAN BE, FOR INSTANCE, GIVEN BY A CURVE DESCRIBED BY THE PARAMETRIC EQUATION:

$$C: \begin{cases} x = x(t) \\ y = y(t) \end{cases} \quad t \in (t_1, t_2)$$



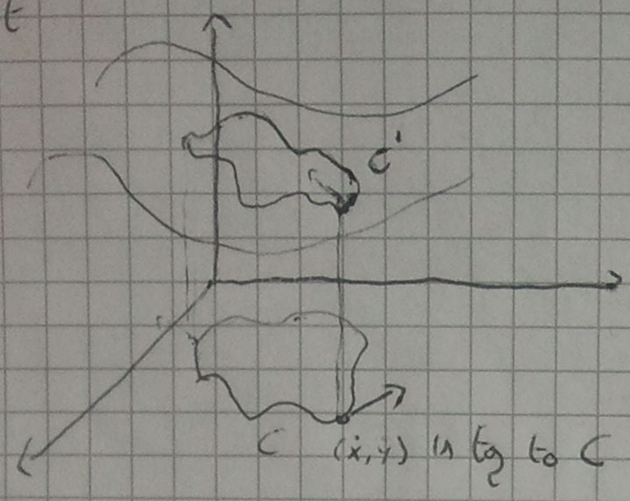
C' GIVEN BY THE SET OF POINT

$$\big(x(t), y(t), F(t) = f(x(t), y(t))\big)$$

Now, the extrema on C' can be calculated by

$$\frac{dF(t)}{dt} = 0$$

$\frac{dF}{dt} = \nabla f \cdot (\dot{x}, \dot{y})$

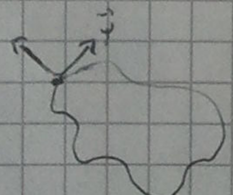


$\frac{dF}{dt} = 0$ IF $\vec{\nabla} f \perp (\dot{x}, \dot{y})$.

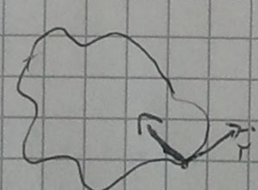
ON THE OTHER HAND, WHAT IS $\vec{\nabla} f$ ON THE PLANE? FOR A GIVEN POINT, $\vec{\nabla} f$ IS THE DIRECTION ALONG WHICH THE CURVE RISES MOST!

OBVIOUSLY, WHEN $\vec{\nabla} f \perp (\dot{x}, \dot{y})$ WE HAVE AN EXTREMUM FOR C'.

IN PARTICULAR:



MAXIMUM ON C'
(DIRECTED
OUTSIDE)



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$\vec{\nabla} f$ HAS INDEED TWO MEANINGS... AS TG VIA $(a, b, (a,b) \cdot \vec{\nabla} f)$ (a VECTOR IN 3D)

AS THE FASTEST INCREASE as $\vec{\nabla} f$ (VECTOR IN 2D)

GENERAL TO N DIMENSIONS IS POSSIBLE AND STRAIGHTFORWARD.

ON THE OTHER HAND, THE CONSTRAINT-CURVE C CAN BE ALSO EXPRESSED IN AN IMPLICIT WAY:

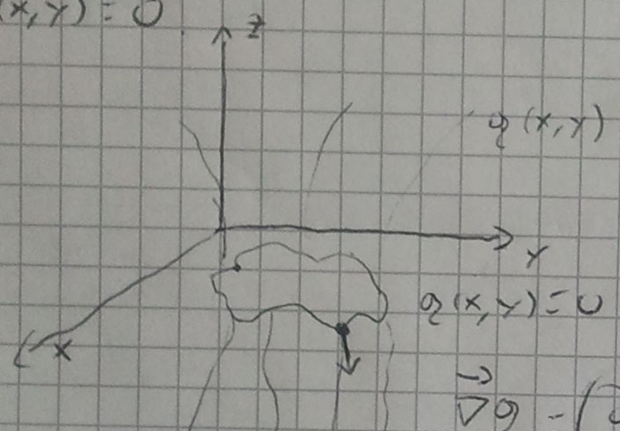
$$C: \begin{cases} x = x(t) \\ y = y(t) \end{cases} \longleftrightarrow g(x,y) = 0.$$

WE HAVE

$f(x,y)$

AND THE CONSTRAIN

$C: g(x,y) = 0$



$g(x,y) = 0$ defines C.

$$\vec{\nabla} g = \left(\frac{\partial g}{\partial x}, \frac{\partial g}{\partial y} \right)$$

Namely:

$$\underset{\forall t}{g(x(t), y(t)) = 0} = \vec{\nabla} g \cdot (\dot{x}(t), \dot{y}(t))$$

Ergo, by construction $\vec{\nabla} g$ is $\perp$ to $\dot{\gamma}$ $\perp$ to the curve C. $\vec{\nabla} g$ is always $\perp$ to $\dot{\gamma}$ for each point on C.

Ergo, it follows that for an extremum on C we must have that:

$$\vec{\nabla} f \cdot \vec{\dot{\gamma}} = 0 \rightarrow \vec{\nabla} f \parallel \vec{\nabla} g$$

$$\vec{\nabla} f = \lambda \vec{\nabla} g$$

WHERE λ IS A CONSTANT (LAGRANGE MULTIPLIER).

WE THEN CONSTRUCT THE FUNCTION

$$\eta(x, y, \lambda) = f(x,y) - \lambda g(x,y)$$

$\lambda \downarrow$ NEW VARIABLE

AND WE SEARCH FOR AN EXTREMUM OF $\eta(x, y, \lambda)$.

THIS BRINGS TO:

$$\partial_x \eta = 0 = \partial_x f - \lambda \partial_x g = 0$$
$$\partial_y \eta = 0 = \partial_y f - \lambda \partial_y g = 0$$

$\Rightarrow \vec{\nabla} f = \lambda \vec{\nabla} g$

$$\partial_\lambda \eta = 0 = g(x,y)$$

$\rightarrow$ the constraint C.

BACK TO PHYSICS: ENTROPY, STATISTICAL OPERATOR, THERMODYNAMICAL POTENTIAL

FOR A CERTAIN PROBLEM WE HAVE AN HILBERT SPACE

$$\mathcal{F} = \{ |m, k_1, \dots, k_N\rangle \}$$

WITH THE EIGENVALUES OF $H, Q_1, \dots, Q_N$ WITH $\begin{cases} [H, Q_i] = 0 \\ [Q_i, Q_j] = 0 \end{cases}$.

(EVENTUAL CONSTRAINTS ARE ALREADY TAKEN INTO ACCOUNT AND ARE NOT PART OF $\mathcal{F}$. FOR INSTANCE, IN THE MICROCANONICAL ENSEMBLE THE ENERGY IS FIXED).

THE PARTITION FUNCTION (IN ITS MOST GENERAL FORM) IS GIVEN BY:

$$Z(\beta, \gamma_1, \dots, \gamma_N) = \sum_{m, k_1, \dots, k_N} \langle m, k_1, \dots, k_N | e^{-\beta H - \gamma_1 Q_1 - \dots - \gamma_N Q_N} | m, k_1, \dots, k_N \rangle$$

A CERTAIN PHYSICAL SITUATION IS REALIZED FOR A PARTICULAR CHOICE $(\beta_0, \gamma_{1,0}, \dots, \gamma_{N,0})$.

THE AVERAGES ARE GIVEN BY:

$$\langle E \rangle = -\partial_\beta \ln Z \Big|_{\beta_0, \gamma_{1,0}, \dots, \gamma_{N,0}} \quad ; \quad (\Delta E)^2 = \frac{\partial^2}{\partial \beta^2} \ln Z \Big|_{\beta_0, \gamma_{1,0}, \dots, \gamma_{N,0}}$$

$$\langle Q_i \rangle = -\partial_{\gamma_i} \ln Z \Big|_{\beta_0, \gamma_{1,0}, \dots, \gamma_{N,0}} \qquad (\Delta Q_i)^2 = \frac{\partial^2}{\partial \gamma_i^2} \ln Z \Big|_{\beta_0, \gamma_{1,0}, \dots, \gamma_{N,0}}$$

THE PROBABILITY THAT THE SYSTEM IS DESCRIBED BY THE STATE

$|m, \lambda_1, \dots, \lambda_N\rangle$

IS GIVEN BY

$$P_{|m,\lambda_1,\dots,\lambda_N\rangle} = \left. \frac{e^{-\beta E_m - \gamma_1 q_{1,\lambda_1} - \dots - \gamma_N q_{N,\lambda_N}}}{Z} \right|_{\beta_0, \gamma_{1,0}, \dots, \gamma_{N,0}}$$

NOW, WE WOULD LIKE TO SHOW THAT THESE PROBABILITIES MAXIMIZE THE ENTROPY ACCORDING TO THE CONSTRAINTS ON THE SYSTEM.

$$S = -k_B \sum_{m,\lambda_1,\dots,\lambda_N} P_{|m,\lambda_1,\dots,\lambda_N\rangle} \ln P_{|m,\lambda_1,\dots,\lambda_N\rangle} \qquad [k_B = 1]$$

MAXIM. OF ENTROPY

SUPPOSE THAT WE DONOT KNOW THE PROBABILITIES YET...

$$S = -\sum_{m,k_1,\ldots,k_N} P_{|m,k_1,\ldots,k_N>} \ln P_{|m,k_1,\ldots,k_N>}$$

IS A FUNCTION THAT WE WANT MAXIMIZE

HOWEVER, WE HAVE CONSTRAINTS:

$$\sum_{m,k_1,\ldots,k_N} P_{|m,k_1,\ldots k_N>} = 1$$

$$<E> = \sum_{m,k_1,\ldots,k_N} P_{|m,\ldots>} E_m$$

$$<Q_1> = \sum_{m,k_1,\ldots,k_N} P_{|m,\ldots>} q_{1,k_1}$$

are fixed.

THEN, WE HAVE TO MAXIMIZE THE FUNCTION

$$S - (\alpha - 1)\left(\sum P_{|m,\ldots>} - 1\right) - \beta\left(\sum P_{|m,\ldots>} E_m - <E>\right)$$
$$- \sum_{i=1}^{N} \gamma_i \left(\sum P_{|m,\ldots>} q_{i,k_i} - <Q_i>\right) = F(P_{|m,\ldots>}, \underbrace{\alpha, \beta, \gamma_i}_{\text{extra-parameters}})$$

$\alpha, \beta, \gamma_1, \ldots, \gamma_N$ ARE LAGRANGE MULTPLIERS...

IN ORDER TO HAVE COMPACT EXPRESSION WE DEFINE THE STATISTICAL OPERATOR AS:

$$\hat{\rho} = \sum_{m,k_1,\dots,k_N} P_{|m,k_1,\dots,k_N\rangle} |P_{m,k_1,\dots,k_N}\rangle\langle P_{m,k_1,\dots,k_N}|$$

$\hat{\rho}$ depends also on $P_{|m,k_1,\dots,k_N\rangle}$ and is such that:

$$Tr[\hat{\rho}] = 1$$

$$\langle E\rangle = Tr[H\hat{\rho}] = \langle H\rangle$$

$$\langle Q_i\rangle = Tr[Q_i\hat{\rho}]$$

$$S = -Tr[\hat{\rho}\ln\hat{\rho}] = -\langle\ln\hat{\rho}\rangle$$

Ergo, we have to maximize

$$-Tr[\hat{\rho}\ln\hat{\rho}] - (\alpha-1)(Tr[\hat{\rho}]-1) - \beta(Tr[H\hat{\rho}]-\langle E\rangle) - \gamma_i(Tr[\hat{\rho}Q_i]-\langle Q_i\rangle)$$

$$= -Tr\{\hat{\rho}\ln\hat{\rho} + (\alpha-1)\hat{\rho} + \beta H\hat{\rho} + \gamma_i Q_i\hat{\rho}\} + \underbrace{\dots}_{\text{indip. on } P_{|\dots\rangle}}$$

WE DERIVE WITH RESPECT TO $\hat{\rho}$.

$$= -Tr[\ln\hat{\rho} + 1 + \alpha - 1 + \beta H + \gamma_i Q_i] = 0$$

$$\ln\hat{\rho} + \alpha + (\beta H + \gamma_i Q_i) = 0$$

$$\hat{\rho} = e^{-\alpha} e^{-\beta H - \gamma_i Q_i}$$

Then USING THE CONSTRAINT: $\mathrm{Tr}[\hat{\varrho}] = 1$

$$\mathrm{Tr}[\hat{\varrho}] = e^{-\alpha}\,\mathrm{Tr}\left[e^{-\beta H - \gamma_i Q_i}\right] = 1 \mapsto e^{-\alpha} = \frac{1}{\mathrm{Tr}\left[e^{-\beta H - \gamma_i Q_i}\right]}$$

Ergo:

$$\hat{\varrho} = \frac{e^{-\beta H - \gamma_i Q_i}}{\mathrm{Tr}\left[e^{-\beta H - \gamma_i Q_i}\right]}$$

$$P_{|m, \lambda_1, \ldots \lambda_N\rangle} = \langle m, \lambda_1, \ldots, \lambda_N | \hat{\varrho} | m, \ldots, \lambda_1, \ldots, \lambda_N\rangle = \frac{\langle m, \lambda_1, \ldots, \lambda_N | e^{-\beta H - \gamma_i Q_i} | m, \lambda_1, \ldots, \lambda_N\rangle}{Z}$$

with $Z = \mathrm{Tr}\left[e^{-\beta H - \gamma_i Q_i}\right] = \sum_{m, \lambda_1, \ldots, \lambda_N} \langle m, \lambda_1, \ldots, \lambda_N | e^{-\beta H - \gamma_i Q_i} | m, \lambda_1, \ldots, \lambda_N\rangle.$

EQUIVALENTLY TO THE MAXIMIZATION OF ENTROPY, ONE CAN STUDY THE MINIMIZATION OF

$$\gamma_i \,\mathrm{Tr}[\hat{\varrho} Q_i] + \beta\,\mathrm{Tr}[\hat{\varrho} H] + (\alpha - 1)\sum_m P_m - S$$

BY DIVIDIGN BY $\beta = 1/T$ WE THEN FIND THAT WE HAVE TO MINIMIZE THE SO-CALLED TERMOD. POTENTIAL

$$\Omega = \mathrm{Tr}[\hat{\varrho} H] + \frac{\gamma_i}{\beta}\mathrm{Tr}[\hat{\varrho} Q_i] - TS$$ (WHERE $\sum_m P_m = 1$ has been used).

Ergo:

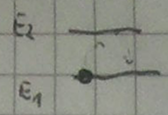
$$\Omega = \langle E \rangle - \mu_i \langle Q_i \rangle - TS \quad \text{with } \mu_i = -\frac{\gamma_i}{\beta}$$, μ_i "chemical potentials"

Used very often in TD studies

LINK TO "QUANTUM SUPERPOSITION" AND STATISTICAL OPERATOR $\hat{\varrho}$

Let us consider $\hat{H}$ only with basis $\{|E_1\rangle, |E_2\rangle\}$

In a quantum statistic the probabilities assigned to $|E_1\rangle$ and $|E_2\rangle$ are not quantum probabilities but statistical probabilities.



$P_2 = e^{-\beta E_2}/Z$

$P_1 = \frac{e^{-\beta E_1}}{Z}$

$$\hat{\varrho} = P_1 |E_1\rangle\langle E_1| + P_2 |E_2\rangle\langle E_2| \qquad \varrho \equiv \begin{pmatrix} P_1 & 0 \\ 0 & P_2 \end{pmatrix} \quad \varrho_{nm} = \langle E_n |$$

But suppose that the state of the system is given by the superposition

$$|\psi\rangle = \cos\vartheta |E_1\rangle + \sin\vartheta |E_2\rangle.$$

This is indeed a "quantum superposition" with probabilities (quantum) c^2 and s^2 to find $|E_1\rangle$ or $|E_2\rangle$ "respectively.

The statistical operator is "defined as" $\hat{\varrho} = |\psi\rangle\langle\psi|$

if we calculate the elements we get:

$$\langle E_1|\hat{\varrho}|E_1\rangle = |\langle E_1|\psi\rangle|^2 = c^2$$

$$\langle E_2|\hat{\varrho}|E_2\rangle = |\langle E_2|\psi\rangle|^2 = s^2$$

$$\langle E_1|\hat{\varrho}|E_2\rangle = \langle E_1|\psi\rangle\langle\psi|E_2\rangle = s \cdot c$$

$$\langle E_2|\hat{\varrho}|E_1\rangle = \langle E_2|\psi\rangle\langle\psi|E_1\rangle = s \cdot c$$

$$\varrho = \begin{pmatrix} c^2 & sc \\ sc & s^2 \end{pmatrix}$$

→ "indicates the presence of a quantum superposition".

c^2 and s^2 are probabilities, but are "quantum prob."

The interaction with an apparatus measuring the energy can generate the phenomenon of "decoherence" which de facto almost eliminates the non-diagonal elements.

How, care is needed:

- $\hat{\varrho}$ in presence of QM is a rather different concept, as we result from quantum superpositions.

- Along which basis should $\hat{\varrho}$ become diagonal?

Still, upon measurement of the energy:

$$\underbrace{|\Psi_{TOT}\rangle = |\psi\rangle|D_0\rangle}_{\text{before meas.}} \longmapsto \underbrace{c|E_1\rangle|D_1\rangle + s|E_2\rangle|D_2\rangle = |\Psi_{tot}\rangle}_{\text{after meas.}}$$

huge "dfs"

superposition of macroscopic distinct worlds

$$\hat{\varrho}_{tot} = |\Psi_{tot}\rangle\langle\Psi_{tot}|$$

$$\hat{\varrho}_{red} = \underset{\substack{\text{all} \\ \text{but } |\psi\rangle}}{\mathrm{Tr}}[\hat{\varrho}] = \langle D_1|\hat{\varrho}_{tot}|D_1\rangle + \langle D_2|\hat{\varrho}_{tot}|D_2\rangle =$$

$$= (c|E_1\rangle + s|E_2\rangle\langle D_1|D_2\rangle)(c\langle E_1| + s\langle E_2|\langle D_2|D_1\rangle)$$
$$+ (c|E_1\rangle\langle D_2|D_1\rangle + s|E_2\rangle)(c\langle E_1|\langle D_1|D_2\rangle + s\langle E_2|)$$

$$|D_0\rangle \text{ evolves to } \begin{cases} |D_1\rangle \\ |D_2\rangle \end{cases} \qquad \langle D_1|D_2\rangle \simeq 0 \quad \text{(but not exactly zero)}$$

$$\varrho_{red} = \begin{pmatrix} c^2 & 0 \\ 0 & s^2 \end{pmatrix} \qquad \text{for } \langle D_1|D_2\rangle \simeq 0$$

To take into account that ...

difficult calculation whose final outcome is

$$\rho_{red} = \begin{pmatrix} c^2 & \langle D_1 | D_2 \rangle \\ \langle D_2 | D_1 \rangle & s^2 \end{pmatrix} \simeq \begin{pmatrix} c^2 & 0 \\ 0 & s^2 \end{pmatrix}$$

STILL, THE PROBLEMS OF QM ARE NOT SOLVED .. THE WHOLE STATE IS STILL IN A SUPERPOSITION.