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Second order differentiability of integral functionals on Sobolev spaces and L^2 -spaces

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1. Introduction

Let Ω be a domain in \mathbb{R}^d , and consider an integral functional f of the form

(1.1)
$$f(u) = \int_{\Omega} \phi(x, u(x), \mathbf{D}u(x)) dx, \quad u \in W_2^1(\Omega)$$

on the Sobolev space $W_2^1(\Omega)$. Here $\mathbf{D} = \left(\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_d}\right)$ and $\phi: \Omega \times \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$ is measurable and satisfies a growth condition of the form

$$|\phi(x, u, p)| \le C(u^2 + |p|^2) + g(x)$$

for some $g \in L^1(\Omega)$, a.a. x, and all u, p. Suppose ϕ is of class C^2 in u, p and the second partial derivatives are uniformly bounded, i.e.,

(1.3)
$$\left| \frac{\partial^2 \phi(x, u, p)}{\partial u^2} \right|, \left| \frac{\partial^2 \phi(x, u, p)}{\partial u \partial p_i} \right|, \left| \frac{\partial^2 \phi(x, u, p)}{\partial p_i \partial p_i} \right| \leq K < \infty$$

for some K > 0 and a.a. $x \in \Omega$ and all u, p. It follows that f is a function of class C^1 on the Hilbert space $W_2^1(\Omega)$. Is it true that f is of class C^2 ? This need not be the case in general, (see [23] or [9], p. 98, for a discussion). We give an explicit example in Section 2. Actually, we can say much more, namely, a result of Nemirovski and Semenov [15], p. 276, tells (roughly) that the functions f of class C^2 constitute only a little band among the integral functionals f. More precisely, their result states that a functional (1.1)-(1.2) is of class C_u^2 only when $\phi(x, u, p)$ is a polynomial of degree ≤ 2 in u, p. (Here C_u^2 means the functions of class C^2 whose second derivative is uniformly continuous on bounded sets.)

The reason why a functional f satisfying (1.1)-(1.3) may fail to be of class C^2 lies in the fact that C^2 refers to differentiability of ∇f in the Fréchet sense and to norm to norm continuity of the Hessian operator. Indeed, our present discussion shows that using Gâteaux differentiability instead leads to a positive result, i.e., ∇f is everywhere Gâteaux differentiability

able, and the Hessian operator $\nabla^2 f$ is norm to weak continuous (Theorems 4.2, Corollary 5.2). However, if the functional (1.1)–(1.3) is considered as a function on $W_2^{\ell}(\Omega)$, where $\ell > d/2 + 1$ and the domain Ω allows for the embedding theorem, then f turns out to be everywhere second order differentiable in the Fréchet sense, but not necessarily of class C^2 (Theorem 5.4).

Now let f be a functional satisfying (1.1), (1.2), but not necessarily (1.3). Is it true that f has a second Gâteaux derivative at those $u \in W_2^1(\Omega)$ where

$$(1.4) |\mathbf{D}^{\alpha}\phi(x,u(x),\mathbf{D}u(x))| \leq K < \infty, |\alpha| = 2 \text{ for a.a. } x \in \Omega$$

is satisfied? In view of the above result it comes as a surprise that the answer is in the negative (Example 2.3), i.e., the boundedness condition (1.4) at u alone does *not* guarantee second order differentiability at u in the Gâteaux sense.

Let f satisfy (1.1), (1.2) and have integrand $\phi(x, u, p)$ of class C^2 in u, p. Is it true that f is at least *densely* second order differentiable? We show that the answer is in the positive e.g. for convex f, or more generally, in the case where the eigenvalues of the Hessian matrices $\nabla^2 \phi(x, u(x), \mathbf{D}u(x))$ are essentially uniformly bounded below (resp. above). More precisely, in these cases, ∇f is Gâteaux differentiable at the points u of a dense subset of $W_2^1(\Omega)$.

Intuitively, a functional f satisfying (1.1), (1.2) is *close* to twice differentiable at u when (1.4) is satisfied. We even know what the Hessian operator $\nabla^2 f(u)$ should look like, namely

$$(1.5) \quad \langle \nabla^2 f(u)h, h \rangle_{W_2^1(\Omega)} = \int_{\Omega} \langle \nabla^2 \phi(x, u(x), \mathbf{D}u(x)) (h(x), \mathbf{D}h(x)), (h(x), \mathbf{D}h(x)) \rangle dx,$$

 $h \in W_2^1(\Omega)$. Here we present a notion of a generalized second derivative which appeals to this context, i.e., it may be helpful in situations where the second Gâteaux derivative fails to exist, but the generalized Hessian operator (1.5) is defined. Our approach is motivated by the notion of second epi derivatives, used by R.T. Rockafellar [21], [22] in finite dimensions. For convex functions f, these have been extended to Hilbert space by J. Borwein and the author [5], § 6. Second epi derivatives are part of the theory of graphical convergence. See [1], [2], [3], [4], [5], [12] for an overview on this.

Besides integral functionals (1.1)-(1.3) on spaces W_2^m we also consider integral functionals on spaces L^2 (see Section 3). The results we obtain are completely analoguous for both types of functionals, so we prefer to use L^2 functionals as prototypes in the principal Sections 3, 4.

2. Second derivatives

In this section we discuss the basic notions of differentiability needed in this work.

Let f be a continuous real-valued function defined on some Hilbert space H. For the notion of a Fréchet resp. Gâteaux derivative of f at x we refer to [9], [10]. The function f is of class C^1 on an open set U if f is Fréchet differentiable on U and the derivative ∇f is norm to norm continuous on U.

Concerning second derivatives of f, we consider convergence of the difference quotient

(2.1)
$$\frac{1}{t} (\nabla f(x+th) - \nabla f(x)) \rightarrow T_x h \quad (t \rightarrow 0),$$

of ∇f at x to some bounded symmetric linear operator T_x on H. We use the notation $T_x = \nabla^2 f(x)$, calling T_x the Hessian of f at x. There are at least four different ways in which convergence of (2.1) may be understood.

We say that f is second order Gâteaux differentiable at x resp. weakly second order Gâteaux differentiable if convergence (2.1) is pointwise in h with respect to the norm topology resp. pointwise in h with respect to the weak topology. On the other hand, f is called second order Fréchet differentiable resp. weakly second order Fréchet differentiable at x when convergence in (2.1) is uniform on $||h|| \le 1$ and in the norm topology resp. uniform on $||h|| \le 1$ and in the weak topology. f is said to be of class C^2 on an open set f if it is of class f and is second order Fréchet differentiable on f and the operator f is norm to norm continuous.

There are four obvious implications among the four notions of second order differentiability, none of which may be reversed in general. We focus on one situation where one of the implications may be reversed.

Proposition 2.1 (cf. [5], Prop. 3.2). Let H be a separable Hilbert space. Let f be first order Gâteaux differentiable in a neighbourhood of x and suppose f is weakly second order Gâteaux differentiable at x. Suppose that ∇f is directionally weakly absolutely continuous in a neighbourhood of x, i.e., $t \to \langle \nabla f(x+th), k \rangle$ is absolutely continuous for small t and fixed h, k. Then f is in fact second order Gâteaux differentiable at x, i.e., weak convergence in (2.1) may be improved to norm convergence.

There is an alternative way of looking at second order differentiability which avoids using the difference quotient (2.1) of ∇f . This is motivated by the study of convex functions f, where one wishes to discuss second order notions without having a first order derivative in the above sense (see [5]) at all points. Namely we take the second difference quotient of f at x with respect to some $y \in H$,

(2.2)
$$\Delta_{f,x,y,t}(h) = \frac{f(x+th) - f(x) - t\langle y, h \rangle}{t^2},$$

considered as a function of h for every fixed $t \neq 0$. Notice that y will usually be the gradient $\nabla f(x)$ here, or more generally a generalized gradient $y \in \partial f(x)$ in the sense of convex analysis or a Clarke generalized gradient [8] when f is a locally Lipschitz function.

A function $q: H \to \mathbb{R}$ is called *purely quadratic* if it has a representation of the form

(2.3)
$$q(h) = \frac{1}{2} \langle Th, h \rangle, \quad h \in H$$

for a bounded and symmetric linear operator $T \in \mathcal{L}(H)$. With these preparations we may now discuss convergence of the second difference quotient (2.2) at x to some purely quadratic limit function q_x as $t \to 0$. Naturally, this is the same as asking whether, in some sense or other, f admits a second order Taylor expansion at x. Again, there are various possible notions of convergence of (2.2) here, for instance, we may consider pointwise convergence, or uniform convergence on compact resp. bounded sets.

Definition 2.1. We write $x \in D_f^2$ if the second difference quotient (2.2) converges uniformly on compact sets to some purely quadratic limit function q_x .

This agrees with our notation from [5], § 2, where we defined D_f^2 for convex f to be the set of points x where f has a pointwise second order Taylor expansion, i.e., where (2.2) converges pointwise. Indeed, since for convex f the second difference quotient is a convex function of h, we may invoke Arzela-Ascoli to improve pointwise convergence to uniform convergence on compact sets. Notice, however, that in infinite dimensions, we do not get uniform convergence on bounded sets. For examples see [5], § 3.

The existence of a second order Taylor expansion is generally weaker than second order differentiability. However, for convex functions, J. Borwein and the author ([5], §3) have shown that $x \in D_f^2$ is equivalent to pointwise weak convergence of the difference quotient $\frac{1}{t}(\partial f(x+th)-\partial f(x))$ as $t\to 0$, i.e., to second order weak Gâteaux differentiability of f at x, while uniform convergence of (2.2) on bounded sets corresponds to second order Fréchet differentiability. Naturally, the same observations pertain to functions f+g with f convex, g of class C^2 . In particular, this is the case for the integral functionals with C^2 integrand satisfying (1.1)-(1.3).

Let us now focus on different types of convergence of (2.2) which are familiar in the context of graphical convergence of functions.

We consider real-valued (or more generally extended real valued) functions f_n , f on H. The sequence (f_n) said to *epi converge* to the limit f if the following conditions are satisfied:

- (a) Given any $x \in H$, there exist $x_n \to x$ (norm) such that $f_n(x_n) \to f(x)$.
- (β) Given any $x \in H$, a sequence $n_k \nearrow \infty$ of indices and a sequence $x_k \to x$ (norm), we have $f(x) \le \lim_{k \to \infty} f_{n_k}(x_k)$.

The sequence (f_n) is said to *Mosco converge* to the limit f if conditions (α) and $(\tilde{\beta})$ are satisfied, where:

($\tilde{\beta}$) Given any $x \in H$, a sequence $n_k \nearrow \infty$ of indices, and a sequence $x_k \rightarrow x$ (weakly), we have $f(x) \le \lim_{k \to \infty} f_{n_k}(x_k)$.

Compare [1], [2] for these notions. We use the notations $f_n \xrightarrow{e} f$ resp. $f_n \xrightarrow{m} f$. Clearly Mosco convergence entails epi convergence, and both notions coincide in finite

dimensions. As was already observed in [3], Mosco convergence $f_n \xrightarrow{m} f$ does not lead to a reasonable concept unless the functions f_n , f are weakly lower semi continuous. For suppose f is not weakly lower semi-continuous, then the constant sequence $f_n = f$ fails to converge to the limit f. Therefore, essentially, the use of Mosco convergence is limited to the case of convex functions. Similarly, epi convergence requires functions which are lower semi-continuous with respect to the norm, but this is a natural requirement even when the functions under consideration are not necessarily convex.

Definition 2.2. The continuous function f on H has a generalized second derivative at $x \in H$ if there exists a purely quadratic function q_x such that the second difference quotient $\Delta_{f,x,y,t}$ epi converges to q_x as $t \to 0$, $(y = \nabla f(x))$. The operator T_x associated with q_x as in (2.3) is called the generalized Hessian of f at x, noted $T_x = \nabla^2 f(x)$. We use the notation $x \in GD_f^2$ if f has a generalized second derivative at x.

Compare [21], [22] and [16], where generalized second derivatives in the sense of Definition 2.2 have been discussed in finite dimensions. Observe that epi convergence $\Delta_{f,x,y,t} \xrightarrow{e} q_x$ entails that y is the gradient of f at x.

Notice that in [5], § 6, we used Mosco convergence to introduce the notion of a generalized second derivative for convex functionals on Hilbert space, while the present approach is based on epi convergence as the defining notion of convergence. This is enforced since using Mosco convergence in the non-convex case is out of the question. But then we end up with two concurring concepts of a generalized second derivative in the convex case. Fortunately, as we will see in Section 3 (Corollary 3.2), both notions coincide at least for convex integral functionals.

It can be shown that $D_f^2 \subset GD_f^2$, see [5], Prop. 6.1, or [16]. Also notice that $GD_f^2 \cap GD_{-f}^2 \subset D_f^2$, i.e. if f and -f both have a generalized second derivative at x, then f has a second order Taylor expansion at x. This may be checked using conditions (α) and (β). Therefore, the generalized second derivative may be understood as a one-sided second derivative.

We end this section with some examples illustrating the interrelation between the various types of second derivatives and generalized second derivatives.

Example 2.1. Let $\Omega=(0,1)$. For $\tau\in\Omega$ define an even convex C^2 function $\phi(\tau,\cdot)$ by $\phi(\tau,x)=\tau^{-1/4}|x|$ for $|x|\geq \tau^{-1/4}$, and $\phi(\tau,x)=-\frac{1}{8}\tau^{1/2}x^4+\frac{3}{4}x^2+\frac{3}{8}\tau^{-1/2}$ for $|x|\leq \tau^{-1/4}$. Notice that $\phi(\tau,x)$ is measurable, and that $\tau\to\phi(\tau,x(\tau))$ is an L^1 function for every $x\in L^2$. We may therefore define a convex integral functional f on $L^2(1,\infty)$ by

$$f(x) = \int_0^1 \phi(\tau, x(\tau)) d\tau.$$

By Theorem 4.2, f has a second Gâteaux derivative q_x at every $x \in L^2$, i.e. $D_f^2 = L^2$. Indeed, we have $0 \le \phi''(\tau, x) \le \frac{3}{2}$, hence $q_x(h) = \int_0^1 \phi''(\tau, x(\tau)) h(\tau)^2 d\tau$ is defined on $L^2(0, 1)$. However, f fails to be of class C^2 . In fact, f is not second order Fréchet differentiable at any

 $x \in L^2$. This may be seen from [23] or proved directly. Let us show exemplarly that ∇f is not Fréchet differentiable in norm at x = 0.

For $\delta > 0$ let $h^{\delta} \in L^2$ be defined by $h^{\delta}(\tau) = \tau^{-1/4}$ for $\tau < \delta$, $h^{\delta}(\tau) = 0$ else. Then we have

$$\langle \nabla f(x+h^{\delta}) - \nabla f(x) - \nabla^2 f(x) h^{\delta}, h^{\delta} \rangle = \int_0^{\delta} \left(\tau^{-1/4} - \frac{3}{2} \tau^{-1/4} \right) \tau^{-1/4} d\tau = -\frac{1}{2} \|h^{\delta}\|^2.$$

But norm Fréchet differentiability of ∇f at x = 0 would require this term to be of the form $\mathcal{O}(\|h^{\delta}\|^2)$ as $\delta \to 0$. This proves the claim.

Notice also that $\nabla^2 f$ is norm to weak continuous, but fails to be norm to norm continuous at any x here.

Example 2.2. The above example may be modified so that $\phi(\tau, x)$ is even of class C^{∞} with bounded ϕ'' and such that $\phi(\tau, x) = \tau^{-1/4}|x|$ for $|x| \ge \tau^{-1/4}$.

Example 2.3. We give an example showing that (1.1), (1.2) and (1.4) does not yield second order differentiability of f at a given point.

Let $\Omega = (1, \infty)$, and define $\phi(\tau, x)$ by $\phi(\tau, x) = \tau^{-\alpha}|x|$ for $|x| \ge \tau^{-2}$, $(1/2 < \alpha < 1$ fixed), and $\phi(\tau, \cdot)$ smooth and convex on $[-\tau^{-2}, \tau^{-2}]$. Let f be the convex integral functional with integrand ϕ .

Let $x \in L^2$ be $x(\tau) = \tau^{-2}$. Then f has a generalized second derivative at x, namely $q_x = 0$, i.e., $x \in GD_f^2$. This follows from Corollary 3.2. However, we have $x \notin D_f^2$, i.e., f is not even second order weakly Gâteaux differentiable at x. Indeed, according to [5], Prop. 2.2, $x \in D_f^2$ would imply that f is Lipschitz smooth at x in the sense of [11], [6], i.e., there would exist C > 0 and $\delta > 0$ such that

$$f(x+h) - f(x) - \langle \nabla f(x), h \rangle \le C ||h||^2$$

is satisfied for all $||h|| \le \delta$. We show that this is not the case. Indeed, define h^{δ} by $h^{\delta}(\tau) = -\tau^{-1}$ for $\tau \ge \delta^{-1}$, $h^{\delta} = 0$ else. Then we have

$$f(x+h^{\delta}) - f(x) - \langle \nabla f(x), h^{\delta} \rangle = \int_{\delta^{-1}}^{\infty} \tau^{-\alpha} (|\tau^{-2} - \tau^{-1}| - \tau^{-2}) + \tau^{-\alpha} \tau^{-1} d\tau$$
$$= \mathcal{O}(\delta^{2\alpha}) + \mathcal{O}(\delta^{2\alpha+2}),$$

which by $1/2 < \alpha < 1$ is not of the form $\mathcal{O}(\|h^b\|^2) = \mathcal{O}(\delta^2)$. So f is not Lipschitz smooth at x.

3. Integral functionals on L^2 -spaces

Let $(\Omega, \mathcal{A}, \mu)$ be a σ -finite measure space, and let $L^2_{R^d}(\Omega, \mathcal{A}, \mu)$ be the Hilbert space of classes of measurable functions $x: \Omega \to \mathbb{R}^d$ having

$$||x||_2 = \left(\int_{\Omega} |x(\tau)|^2(\mu) d\tau\right)^{\frac{1}{2}} < \infty.$$

We consider integral functionals f on $L_{R^d}^2$ of the form

(3.1)
$$f(x) = \int_{\Omega} \phi(\tau, x(\tau))(\mu) d\tau, \quad x \in L^{2}_{R^{d}},$$

with $\phi: \Omega \times \mathbb{R}^d \to \mathbb{R}$ measurable. Clearly, f is convex when $\phi(\tau, x)$ is convex in x. For convenience we assume throughout that f is finite everywhere. This requires a growth condition on $\phi(\tau, x)$, e.g. of the form

$$(3.2) |\phi(\tau, x)| \leq C \cdot |x|^2 + |\langle h(\tau), x \rangle| + g(\tau),$$

for some C > 0 and some $g \in L^1$, $h \in L^2_{R^d}$, see [20]. Also we assume throughout that f is continuous, which holds when $\phi(\tau, x)$ is continuous in x. In particular, this is the case when f is convex. See [20], [23], [9] for basic facts concerning integral functionals.

We start with the following fundamental result on generalized second derivatives. In [5], 6.10, we have obtained a version of this for convex f using duality techniques.

Theorem 3.1. Let f be an integral functional (3.1), (3.2) on L_{Rd}^2 . Suppose $x \in L_{Rd}^2$ satisfies $x(\tau) \in D_{\phi(\tau, \cdot)}^2$ for almost all τ . Then the following statements are equivalent:

- (1) f has generalized second derivative q_x at x;
- (2) $\operatorname{ess\,sup} |\nabla^2 \phi(\tau, x(\tau))| < \infty$, and there exists $\alpha > 0$ such that

(3.3)
$$\Delta_{\phi(\mathfrak{r},\cdot),x(\mathfrak{r}),y(\mathfrak{r}),t}(\xi) + \alpha |\xi|^2 \ge 0$$

for all $0 < |t| \le 1$, all $\xi \in \mathbb{R}^d$, and almost all τ .

Moreover, in these cases, we have the representation

(3.4)
$$q_{x}(h) = \int_{\Omega} \frac{1}{2} \langle \nabla^{2} \phi(\tau, x(\tau)) h(\tau), h(\tau) \rangle \langle \mu \rangle d\tau.$$

Proof. First assume statement (2). Observe that the assumption $x(\tau) \in D^2_{\phi(\tau,\cdot)}$ for a.a. τ implies that there exists a dense subset Φ of $L^2_{R^d}$ such that, for every $h \in \Phi$, the second difference quotient converges pointwise (as $t \to 0$), i.e., $\Delta_t(h) := \Delta_{f,x,y,t}(h) \to q_x(h)$, where q_x is defined as in the statement of the Theorem. Indeed, $x(\tau) \in D^2_{\phi(\tau,\cdot)}$ implies that we find $\delta(\tau) > 0$ such that

(3.5)
$$\left| \Delta_{t}(\tau,\xi) - \frac{1}{2} \langle \nabla^{2} \phi(\tau,x(\tau)) \xi, \xi \rangle \right| \leq 1$$

for all $|\xi| \le 1$ and all $0 < |t| \le \delta(\tau)$. Here we use the notation

$$\Delta_t(\tau,\xi) = \Delta_{\phi(\tau,\cdot),\,x(\tau),\,y(\tau),\,t}(\xi) \; .$$

Also, we may assume that the function $\tau \to \delta(\tau)$ is measurable. Now let (A_m) be an increasing sequence in $\mathscr A$ having $\Omega = \bigcup_{m=1}^{\infty} A_m$, $\mu(A_m) < \infty$. Let

$$E_k = \left\{ \tau \in \Omega : \delta(\tau) \ge \frac{1}{k} \right\},\,$$

then $\Omega \setminus \bigcup_{k=1}^{\infty} E_k$ is a null set by assumption. Now let $\Phi_{m,k,r}$ be the set of functions $h \in L^2_{R^d}$ having $h(\tau) = 0$ for $\tau \notin A_m \cap E_k$, and with $||h||_{\infty} \leq r$. Clearly $\Phi = \bigcup_{m,k,r} \Phi_{m,k,r}$ is dense in $L^2_{R^d}$. We check that, for $h \in \Phi_{m,k,r}$, $\Delta_t(h) \to q_x(h)$. Let $q(\tau,\xi) \coloneqq \frac{1}{2} \langle \nabla^2 \phi(\tau,x(\tau)) \xi, \xi \rangle$, whence $q_x(h) = \int_{\Omega} q(\tau,h(\tau))(\mu) d\tau$. Then (3.5) gives

$$|\Delta_t(\tau, h(\tau))| \leq |q(\tau, h(\tau))| + r^2$$

for the $\tau \in A_m$ and $|t| \leq \delta(\tau)/r$, whence the $\Delta_t(\tau, h(\tau))$ have common integrable majorant $\tau \to (q(\tau, h(\tau)) + r^2) \cdot \chi_{A_m}$. Dominated convergence therefore gives

(3.6)
$$\lim_{t \to 0} \Delta_t(h) = \lim_{t \to 0} \int_{\Omega} \Delta_t(\tau, h(\tau))(\mu) d\tau = \int_{\Omega} \lim_{t \to 0} \Delta_t(\tau, h(\tau))(\mu) d\tau$$
$$= \int_{\Omega} q(\tau, h(\tau))(\mu) d\tau = q_x(h).$$

This proves the statement on Φ .

As a consequence of the observation above we now check condition (α) for the epi convergence $\Delta_t \stackrel{e}{\longrightarrow} q_x$. Indeed, for fixed $h \in L^2_{R^d}$ find $h_m \in \Phi$, $h_m \to h$ in norm. We may assume that $|q_x(h) - q_x(h_m)| \le \frac{1}{m}$. Let a null sequence t_m be fixed. Using $h_m \in \Phi$, we find an increasing sequence k(m) of indices such that

$$|\Delta_{t_n}(h_m) - q_x(h_m)| \le \frac{1}{m}$$

for all $n \ge k(m)$. Define h^r by setting $h^r = h_m$ for $k(m) \le r < k(m+1)$. Then we easily check $\Delta_{t_r}(h^r) \to q(h)$ as $r \to \infty$. This proves condition (a).

Checking condition (β) remains. Let $h_n \to h$ (norm) be fixed. For any null sequence t_n , (3.3) gives

(3.7)
$$\Delta_{t_n}(\tau, h_n(\tau)) + \alpha \cdot |h_n(\tau)|^2 \ge 0$$

for a.a. τ . Select a subsequence $h_{n'}$ such that

$$\underline{\lim}_{n} \left(\Delta_{t_n}(h_n) + \alpha \|h_n\|_2^2 \right) = \lim_{n'} \left(\Delta_{t_{n'}}(h_{n'}) + \alpha \|h_{n'}\|_2^2 \right).$$

Then select another subsequence $h_{n''}$ which converges almost everywhere. By Fatou's Lemma, which applies because of (3.7), we obtain

$$\lim_{n''\to\infty} \left(\Delta_{t_{n''}}(h_{n''}) + \alpha \cdot ||h_{n''}||_2^2\right) \ge \int_{\Omega} \lim_{n''\to\infty} \left(\Delta_{t_{n''}}(\tau, h_{n''}(\tau)) + \alpha \cdot |h_{n''}(\tau)|^2\right) (\mu) d\tau$$

$$= \int_{\Omega} \left(q(\tau, h(\tau)) + \alpha \cdot |h(\tau)|^2\right) (\mu) d\tau.$$

This proves condition (β) , and hence statement (1).

Conversely assume statement (1). Let $\Delta_t \to q$ for a purely quadratic function q. We have to check condition (2) and also $q = q_x$, where q_x has the same meaning as above.

First observe that, by continuity of f, we find $\delta > 0$ such that $|f(x+k)| \le |f(x)| + 1$ for all $||k||_2 \le \delta$. We now claim that there exists $\alpha > 0$ such that, for all $||h||_2 \le \delta$ and $0 < |t| \le 1$, we have

$$(3.8) \qquad \Delta_{\star}(h) + \alpha \cdot ||h||_2^2 \ge 0.$$

Assume the contrary. Then we find $0 < |t_n| \le 1$ and $||h_n||_2 \le \delta$ such that

$$(3.9) \Delta_t (h_n) + n^2 ||h_n||_2^2 < 0$$

for $n=1,2,\ldots$. We have two cases. First assume that, at least for a subsequence, $||h_n||_2 \to 0$. Let σ_n be chosen such that $\sigma_n \nearrow \infty$, $\sigma_n h_n \to 0$ (norm), and $n\sigma_n ||h_n||_2 \to \infty$. Then we have

$$\Delta_{\frac{t_n}{\sigma}}(\sigma_n h_n) = \sigma_n^2 \Delta_{t_n}(h_n) < -n^2 \sigma_n^2 ||h_n||_2^2 \rightarrow -\infty ,$$

a contradiction since $\sigma_n h_n \to 0$ and $t_n/\sigma_n \to 0$, whence $\underline{\lim} \Delta_{\frac{t_n}{\sigma_n}}(\sigma_n h_n) \ge q(0) > -\infty$ by condition (β) . The second case is when $||h_n||_2 \ge \varepsilon > 0$ for every n. Here we necessarily have $t_n \to 0$. Indeed, using (2.1) we have

$$\Delta_{t_n}(h_n) \geq \frac{-2|f(x)|-1-\|\nabla f(x)\|_2 \cdot \delta}{t_n^2},$$

since $||t_n h_n||_2 \le \delta$. But $\Delta_{t_n}(h_n) \to -\infty$ by our assumption (3.9), hence $t_n \to 0$. Now we find a sequence $\varrho_n \to 0$ such that $n\varrho_n^2 \to \infty$ and $t_n/\varrho_n \to 0$. Then we have

$$-n\varrho_n^2 \|h_n\|_2^2 > \varrho_n^2 \Delta_{t_n}(h_n) = \Delta_{\frac{t_n}{\alpha n}}(\varrho_n h_n) ,$$

a contradiction with condition (β) as above, since $\varrho_n h_n \to 0$ (norm). This proves (3.8).

Let us now show that (3.8) implies the second part of the statement (2). Let $\xi \in \mathbb{R}^d$, $\xi \neq 0$ be fixed. We show that for all $0 < |t| \leq 1$ and a.a. τ we have

$$(3.10) \Delta_{r}(\tau,\xi) + \alpha \cdot |\xi|^{2} \geq 0.$$

Assume the contrary, then we find $0 < |t| \le 1$ such that $\{\tau \in \Omega : \Delta_t(\tau, \xi) + \alpha |\xi|^2 < 0\}$ has positive measure. Hence for some $\eta > 0$ the set $\{\tau : \Delta_t(\tau, \xi) + \alpha |\xi|^2 < -\eta\}$ has positive measure. Choose a subset A of this set having $0 < \mu(A) \le \delta/|\xi|$. Let $h = \xi \cdot \chi_A$, where χ_A denotes the indicator function. Then $||h||_2 \le \delta$, so (3.8) gives

$$0 \leq \Delta_t(h) + \alpha ||h||_2^2 = \int_A \left(\Delta_t(\tau, \xi) + \alpha |\xi|^2 \right) (\mu) d\tau \leq -\eta \mu(A) < 0,$$

a contradiction which proves (3.10). Now let (ξ_k) be a dense sequence in \mathbb{R}^d . By the above argument we find for every k a null set N_k such that, for all $0 < |t| \le 1$ and all $\tau \notin N_k$,

$$\Delta_{t}(\tau,\xi_{k}) + \alpha |\xi_{k}|^{2} \geq 0.$$

Let $N = \bigcup_{k} N_k$, then by continuity, we have $\Delta_t(\tau, \xi) + |\xi|^2 \ge 0$ for all $0 < |t| \le 1$, $\tau \notin N$ and all $\xi \in \mathbb{R}^d$. This proves (3.3).

Let us finally check the first part of statement (2). By (3.3) proved before, we clearly have

$$\langle \nabla^2 \phi(\tau, x(\tau)) \xi, \xi \rangle \ge -2\alpha |\xi|^2$$

whence it suffices to find an upper bound for the left hand side here. Fixing h, and using condition (α) , we find $h_m \to h$ (norm) such that, for some fixed null sequence t_m ,

$$\Delta_{t_m}(h_m) \to q(h)$$
.

By Fatou's Lemma, we have

$$(3.11) \quad \lim_{m \to \infty} \left(\Delta_{t_m}(h_m) + \alpha \|h_m\|_2^2 \right) \ge \int_{\Omega} \lim_{m \to \infty} \inf \left(\Delta_{t_m}(\tau, h_m(\tau)) + \alpha |h_m(\tau)|^2 \right) (\mu) d\tau.$$

Selecting a subsequence of h_m which converges almost everywhere, we find that the right hand side in (3.11) equals $\int_{\Omega} \frac{1}{2} \langle \nabla^2 \phi(\tau, x(\tau)) h(\tau), h(\tau) \rangle + \alpha |h(\tau)|^2 (\mu) d\tau$, giving

$$q_x(h) = \int_{\Omega} q(\tau, h(\tau))(\mu) d\tau \leq q(h).$$

As q is bounded above on some open set, we deduce that q_x is continuous, whence $|q_x(h)| \le C < \infty$ for $||h||_2 \le 1$, say. This implies $|q(\tau, \xi)| \le C$ for all $|\xi| \le 1$ and a.a. τ , proving the first part of statement (2).

Finally, to prove $q = q_x$, we use the implication (2) \Rightarrow (1) again, which gives $\Delta_t \xrightarrow{e} q_x$, hence $q = q_x$, since the epi limit of Δ_t is unique. \Box

Remark. The boundedness condition (3.3) does not come as a surprise when we recall that a similar uniform boundedness below condition is required for Mosco convergence of sequences of *convex* functions (see [1], Lemme 1.5).

We obtain an interesting consequence for convex integral functionals. Here we wish to apply results from [5], so we have to assume that the space $L_{R^d}^2$ is separable. This is the case when $\mathscr A$ is countably generated in tandem with our general assumption that μ is σ -finite.

Corollary 3.2. Let f be a convex integral functional (3.1), (3.2.). Suppose $L_{R^d}^2$ is separable. Then for $x \in L_{R^d}^2$ the following statements are equivalent:

- (1) $\Delta_{f,x,y,t} \xrightarrow{e} q_x$ for a purely quadratic convex function q_x .
- (2) $\Delta_{f,x,y,t} \xrightarrow{m} q_x$ for a purely quadratic convex function q_x .
- (3) $x(\tau) \in D^2_{\phi(\tau,\cdot)}$ for almost all τ , and $\operatorname{ess\,sup}_{\tau \in \Omega} |\nabla^2 \phi(\tau, x(\tau))| < \infty$.

Moreover, in these cases, q_x has the representation (3.4).

Proof. The equivalence of (2) and (3) was proved in [5], 6.10, using duality methods. As (2) implies (1), we have but to observe that (1) implies (3) by Theorem 3.1. Indeed, condition (3.3) in statement (2) of the Theorem is automatically satisfied, since

$$\Delta_t(\tau,\cdot) = \Delta_{\phi(\tau,\cdot),t} \geq 0$$

for convex $\phi(\tau, \cdot)$. \Box

- Corollary 3.3. Under the assumptions of Corollary 3.2, let $L^2_{Rd}(\Omega, \mathcal{A}, \mu)$ be such that weak convergence $h_n \rightarrow h$ implies the existence of a subsequence h_n which converges almost everywhere. Then we may include among the list in Theorem 3.1 the following equivalent statement:
- (3) There exists $\alpha > 0$ such that $\Delta_{f,x,y,t} + \alpha \|\cdot\|_2^2 \xrightarrow{m} q_x + \alpha \|\cdot\|_2^2$ for a purely quadratic function q_x .
- Proof. Clearly $\Delta_t + \alpha \|\cdot\|_2^2 \xrightarrow{m} q_x + \alpha \|\cdot\|_2^2$ implies $\Delta_t + \alpha \|\cdot\|_2^2 \xrightarrow{e} q_x + \alpha \|\cdot\|_2^2$, and the latter implies $\Delta_t \xrightarrow{e} q_x$, which is statement (1). Conversely, we have to show that statement (2) of the Theorem implies (3) above. This requires our extra assumption on the space L_{Rd}^2 . We mimick the proof in Theorem 3.1, (2) \Rightarrow (1). The proof of condition (α) remains unchanged. As for condition ($\tilde{\beta}$), let $h_n \to h$ (weakly), then Fatou's Lemma gives the estimate (3.11). Now the extra assumption gives a subsequence which converges almost everywhere, and so the proof proceeds as the proof of Theorem 3.1 did. This completes the argument. \square

Remarks. (1) The extra condition in Corollary 3.3 is valid e.g. in $L_{R^d}^2(\mathbb{N}) = \ell_{R^d}^2$, since here weak convergence entails pointwise convergence. On the other hand the extra condition fails e.g. in $L^2[0,1]$, for here we may exhibit $h_n \rightarrow 0$ weakly such that no subsequence converges a.e. Take $h_n(x) = \sin n\pi x$, then $h_n \rightarrow 0$ by the Riemann-Lebesgue Lemma, but for no subsequence, $h_{n'} \rightarrow 0$ in probability. Indeed, we have

$$\lambda\{x:|h_n(x)|\geq \sqrt{2}/2\}=\frac{1}{2}$$

for every n.

- (2) Let us mention without proof that the extra condition in Corollary 3.3 above may be given an equivalent lattice theoretic formulation. Namely, it holds if and only if the lattice operation $f \to f^+$ is weaky sequentially continuous at 0.
- (3) It might be somewhat surprising that we did not add the statement $\Delta_t \xrightarrow{m} q$ in Corollary 3.3. The reason lies in the fact that the function $\psi = -\alpha \|\cdot\|_2^2$ is not weakly lower semi continuous, so we may not argue that $\phi_n \xrightarrow{m} \phi$ implies $\phi_n + \psi \xrightarrow{m} \phi + \psi$. However, this kind of relation holds when we are dealing with convex functions. Here $\phi_n + \psi \xrightarrow{m} \phi + \psi$ implies $\phi_n \xrightarrow{m} \phi$, and vice versa.

4. Smooth integrands

In this section we discuss the differentiability properties of integral functionals having C^2 -integrand. Concerning first order differentiability resp. class C^1 , the situation is well-known. We have the following

Proposition 4.1. Let f be an integral functional satisfying (3.1), (3.2). Suppose that either $\phi(\tau, x)$ is convex and of class C^1 or that $\phi(\tau, x)$ is of class C^2 and the eigenvalues of the Hessian matrices $\nabla^2 \phi(\tau, x)$ are essentially uniformly bounded below. Then f is of class C^1 on the Hilbert space $L^2_{R^4}$.

Proof. First consider the case where ϕ is convex and of class C^1 . It follows that f is everywhere Gâteaux differentiable and that the operator $\nabla f: L^2_{R^d} \to L^2_{R^d}$ with

$$\nabla f(x)(\tau) = \nabla \phi \left(\tau, x(\tau)\right)$$

is norm to weak continuous. The statement now amounts to proving that ∇f is norm to norm continuous. This follows from a result of Krasnosel'skii (see [10], p. 77).

Now consider the case where ϕ is of class C^2 and where we have

$$\langle \nabla^2 \phi(\tau, \xi) \eta, \eta \rangle \ge -\alpha |\eta|^2$$

for some $\alpha > 0$. This implies convexity of $\phi(\tau, \xi) + \alpha |\xi|^2$, hence the result follows from the first part. \Box

Theorem 4.2. Let f be an integral functional (3.1), (3.2) such that $\phi(\tau, x)$ is of class C^2 in x. Suppose the second partial derivatives of ϕ are essentially uniformly bounded, i.e.,

$$\left|\frac{\partial^2 \phi(\tau, x)}{\partial x_i \partial x_i}\right| \leq K < \infty.$$

Then f is everywhere second order differentiable, i.e. ∇f is everywhere Gâteaux differentiable in norm.

Proof. The assumption (4.1) on $\phi(\tau, x)$ is equivalent to saying that, for some $\alpha > 0$,

(4.2)
$$-\alpha |\xi|^2 \leq \frac{1}{2} \langle \nabla^2 \phi(\tau, \eta) \xi, \xi \rangle \leq \alpha |\xi|^2$$

holds for all ξ , η and a.a. τ . This implies that $\psi(\tau, x) = \phi(\tau, x) + \alpha |x|^2$ is convex. Hence $\Delta_t(\tau, \xi) + \alpha |\xi|^2 \ge 0$, where as usual $\Delta_t(\tau, \xi)$ denotes the second difference quotient of $\phi(\tau, \cdot)$ at $x(\tau)$. Therefore, without loss, we may assume that f is convex.

By (4.2) and Theorem 3.1, f has a generalized second derivative q_x at every $x \in L^2_{R^d}$, i.e., $\Delta_{f,x,y,t} \xrightarrow{e} q_x$. By Corollary 3.2, this is equivalent to $\Delta_{f,x,y,t} \xrightarrow{m} q_x$ for every x.

Now we use our result [5], 6.3, which tells that Mosco convergence $\Delta_{f,x,y,t} \xrightarrow{m} q_x$ implies uniform convergence $\Delta_{f,x,y,t} \to q_x$ on compact sets whenever x is a point of Lipschitz smoothness of f. Denoting the set of Lipschitz smooth points of f by L_f , this reads as $GD_f^2 \cap L_f \subset D_f^2$. But notice that f is Lipschitz smooth at every x, since by (4.1), ∇f is globally Lipschitz with constant K. So $\Delta_{f,x,y,t} \to q_x$ uniformly on compact sets for every x. Notice that, by [5], Thm. 3.1, the latter is equivalent to weak convergence of the difference quotient $1/t(\nabla f(x+th) - \nabla f(x))$ as $(t\to 0)$ for every fixed h and every x. In other words, ∇f is weakly Gâteaux differentiable.

Finally, according to Proposition 2.1, weak convergence of the difference quotient of ∇f may be improved to norm convergence, since ∇f is Lipschitz. This proves the statement. \Box

Remarks. (1) As shown by Example 2.1, we cannot expect ∇f to be densely Fréchet differentiable. See also [5], Ex. 3.3, for a different type of counterexamples.

(2) Notice that, in contrast with the situation in Proposition 5.1, norm to weak continuity of the operator $\nabla^2 f$ cannot be improved to norm to norm continuity, since Krasnosel'skii's result (used in the proof of Proposition 5.1) does not apply to operators mapping into spaces of type L^{∞} (cf. [9]). Indeed, Example 2.1 shows explicitly that $\nabla^2 f$ need not be norm to norm continuous.

Proposition 4.3. Let f be an integral functional (3.1), (3.2) with integrand $\phi(\tau, x)$ of class C^2 . Suppose the eigenvalues of the Hessian matrices $\nabla^2 \phi(\tau, x)$ are essentially uniformly bounded below, i.e., $\phi(\tau, x) + \alpha |x|^2$ is convex for some $\alpha > 0$. Then f is densely second order differentiable, i.e., ∇f is Gâteaux differentiable on a dense set.

Proof. We may assume that f is convex. We invoke a result of Fabian [11], Thm. 2.8, which tells that the L_f of Lipschitz smooth points x of the function f is dense in $L_{R^d}^2$. Now let x be a Lipschitz smooth point of f, i.e., we have

$$f(x+h) - f(x) - \langle \nabla f(x), h \rangle \le C ||h||_2^2$$

for some C > 0, $\delta > 0$, and all $||h||_2 \le \delta$. Now it is clear that this implies that the $\phi(\tau, \cdot)$ as well are Lipschitz smooth at the $x(\tau)$ with the same constant C. In other words,

$$\langle \nabla^2 \phi(\tau, x(\tau)) \xi, \xi \rangle \leq C |\xi|^2$$

since the $\phi(\tau, \cdot)$ are of class C^2 . By Corollary 3.2, f therefore has a generalized second derivative at x. Finally, our result [5], 6.3, implies that f is second order differentiable at such x, i.e., $x \in D_f^2$. To obtain second order Gâteaux differentiability with respect to the norm, we have to use Proposition 2.1, which applies since ∇f is directionally weakly Lipschitz. \Box

5. Integral functionals on Sobolev spaces

In this section we obtain results on second derivatives of integral functionals f satisfying (1.1), (1.2) on a Sobolev space $W_2^1(\Omega)$. Notice that the restriction to integral functionals depending only on first order derivatives is not essential. Similar results for higher derivatives may be obtained with the same techniques.

We start with the following analogue of Theorem 3.1.

Theorem 5.1. Let f be an integral functional (1.1), (1.2). Let $u \in W_2^1(\Omega)$, and suppose $(u(x), \mathbf{D}u(x)) \in D^2_{\phi(x,\cdot,\cdot)}$ for almost all $x \in \Omega$. Then the following statements are equivalent:

- (1) f has a generalized second derivative at u, i.e., $\Delta_{f,u,v,t} \xrightarrow{e} q$ for a purely quadratic function q.
 - (2) $\underset{x \in \Omega}{\text{ess sup}} |\nabla^2 \phi(x, u(x), \mathbf{D} u(x))| < \infty$, and there exists $\alpha > 0$ such that

(5.1)
$$\Delta_{\phi(\mathbf{x},\cdot,\cdot),t}(\xi) + \alpha |\xi|^2 \ge 0$$

for almost all $x \in \Omega$, all $0 < |t| \le 1$ and all $\xi \in \mathbb{R} \times \mathbb{R}^d$.

Moreover, in these cases, we have the representation

$$(5.2) q(h) = \int_{\Omega} \frac{1}{2} \langle \nabla^2 \phi(x, u(x), \mathbf{D} u(x)) (h(x), \mathbf{D} h(x)), (h(x), \mathbf{D} h(x)) \rangle dx.$$

The proof proceeds in much the same way as the proof of Theorem 3.1. We have the following consequence in the spirit of Theorem 4.2.

Corollary 5.2. Let f be an integral functional (1.1), (1.2) on $W_2^1(\Omega)$ such that $\phi(x, u, p)$ is of class C^2 in u, p. Suppose the second partial derivatives of ϕ are essentially bounded, i.e., for a.a. x,

(5.3)
$$\left| \frac{\partial^2 \phi(x, u, p)}{\partial u^2} \right|, \left| \frac{\partial^2 \phi(x, u, p)}{\partial u \partial p_i} \right|, \left| \frac{\partial^2 \phi(x, u, p)}{\partial p_i \partial p_i} \right| \leq C < \infty.$$

Then f is everywhere second order differentiable, i.e., the difference quotient

$$\frac{1}{t} \big(\nabla f(u + th) - \nabla f(u) \big)$$

converges pointwise in norm for every $u \in W_2^1(\Omega)$.

The reasoning is similar to the proof of Theorem 4.2. Notice again that condition (5.3) is equivalent to saying that the eigenvalues of the Hessian operators $\nabla^2 \phi(x, u, p)$ are essentially bounded.

For $\ell \ge 1$, the functional (1.1), (1.2) may be considered as a function on $W_2^{\ell}(\Omega)$. In the following, we assume that the domain Ω allows for the Sobolev embedding Theorems (cf. [24], §8).

Proposition 5.3. Let $\ell > d/2 + 1$, and let f be an integral functional (1.1), (1.2) on the space $W_2^{\ell}(\Omega)$. Let $u \in W_2^{\ell}(\Omega)$ be fixed. Then the following statements are equivalent:

- (1) f has generalized second derivative q_u at u, i.e., $\Delta_{f,u,v,t} \xrightarrow{e} q_u$ in $W_2^{\ell}(\Omega)$.
- (2) $\Delta_{f,u,v,t} \xrightarrow{m} q_u \text{ in } W_2^{\ell}(\Omega).$
- (3) Statement (2) from Theorem 5.1 is satisfied.

Moreover, in these cases, q_u has the representations (5.2).

Proof. We have to show that (3) implies (2). First observe that, for some $\alpha \ge 0$, condition (5.1) gives

$$\Delta_{f,u,v,t} + \alpha \|\cdot\|_{W_2^1}^2 \geq 0.$$

Now we first argue that $\Delta_{f,u,v,t} + \alpha \|\cdot\|_{W_2^1}^2 \xrightarrow{m} q_u + \alpha \|\cdot\|_{W_2^1}^2$. This is the situation from Corollary 3.3. We have to check condition $(\tilde{\beta})$. We take $h_n \to h$ weakly in W_2^ℓ . We get an estimate similar to (3.11), and we need a subsequence h_n such that h_n and $\mathbf{D}h_n$ are both convergent a.e. Now we use the fact that the embedding $W_2^\ell \to L^2$ is compact by $\ell > d/2$ (cf. [24], §8). This gives a subsequence $h_n \to h$ in L^2 -norm, and hence another subsequence which converges a.e. Next we use that because of $\ell + 1 > d/2$ the embedding $W_2^{\ell-1} \to L^2$ as well is compact, hence \mathbf{D} is compact as an operator $W_2^\ell \to L^2$. This provides the subsequence $h_{n''}$ having $\mathbf{D}h_{n''} \to \mathbf{D}h$ a.e. This proves statement $(\tilde{\beta})$.

Let us now show that $\Delta_{f,u,v,t} \xrightarrow{m} q_u$. Again we have but to check $(\tilde{\beta})$. Let $h_n \to h$ weakly in W_2^{ℓ} . Now we argue that h_n has a subsequence which converges in the W_2^1 -norm. But this follows from the compactness of the embedding $W_2^{\ell} \to W_2^1$, the latter being a consequence of the compactness of $W_2^{\ell} \to L^2$ and $W_2^{\ell-1} \to L^2$. \square

We end with the following result which shows that an integral function f satisfying (1.1)-(1.3) is second order differentiable in the Fréchet sense when it is considered as a function on $W_2^{\ell}(\Omega)$ for $\ell > d/2 + 1$, but need not be of class C^2 .

Theorem 5.4. Let f be an integral functional (1.1), (1.2) considered as a function on $W_2^{\ell}(\Omega)$, $\ell > d/2 + 1$. Suppose $\phi(x, u, p)$ has bounded second partial derivatives, i.e., (1.3) is satisfied. Then f is twice differentiable in the Fréchet sense on $W_2^{\ell}(\Omega)$.

Proof. As a consequence of (1.3), we may assume that f is convex. By Corollary 5.1, f is second order Gâteaux differentiable on $W_2^1(\Omega)$, i.e., the second difference quotient $\Delta_{f,u,v,t}$ converges to a purely quadratic limit q_u , with convergence being uniform on compact sets in W_2^1 . Here $v \in \partial f(u)$ is a vector in $W_2^1(\Omega)$. Now observe that the embedding $W_2^\ell \to W_2^1$ is compact as a consequence of $\ell > d/2 + 1$ (cf. [24]). Hence $\Delta_{f,u,v,t}$ converges uniformly on the ball of $W_2^\ell(\Omega)$. Now let $w \in W_2^\ell$ be choosen so that $\Delta_{f|W_2^\ell,u,v,t} = \Delta_{f,u,v,t}|_{W_2^\ell}$. Then we deduce that $\Delta_{f|W_2^\ell,u,v,t}$ converges uniformly on bounded sets in W_2^ℓ . By [5], Thm. 3.1 this implies that $\nabla f|_{W_2^\ell}$ is Fréchet differentiable at $u \in W_2^\ell(\Omega)$. \square

Example 5.1. Let f be the functional from Example 2.3 considered as a function on $W_2^2(0,1)$. Then f is twice differentiable in the Fréchet sense by Theorem 5.4, but $\nabla^2 f$ fails to be norm to norm continuous.

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