Quantum tunneling in deep potential wells and strong magnetic field revisited

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Abstract

Inspired by a recent paper* by Charles Fefferman, Jakob Shapiro and Michael Weinstein, we investigate quantum tunneling for a Hamiltonian with a symmetric double well and a uniform magnetic field. In the simultaneous limit of strong magnetic field and deep potential wells with disjoint supports, tunneling occurs and we derive accurate estimates of its magnitude.

* [Lower bound on quantum tunneling for strong magnetic fields. *SIAM J. Math. Anal.* 54(1), 1105-1130 (2022).]

Presentation

We briefly present what we are looking for.

The Hamiltonian

We start from $\mathfrak{v}_0 \in C_c^\infty(\mathbb{R}^2)$ such that

$$\begin{cases} \mathfrak{v}_0(x) = v_0(|x|) \text{ is radial } \& \ v_0^{\min} := \min\limits_{r \geq 0} v_0(r) < 0\,, \\ \operatorname{supp} \mathfrak{v}_0 \subset \overline{D(0,a)} := \{x \in \mathbb{R}^2 \ : \ |x| \leq a\}\,, \\ U_0 := \{\mathfrak{v}_0(x) = v_0^{\min}\} = \{0\} \quad \& \quad v_0''(0) > 0\,. \end{cases} \tag{1}$$

We suppose that $\overline{D(0,a)}$ is the smallest disc containing $\operatorname{supp} \mathfrak{v}_0$, i.e.

$$a = a(\mathfrak{v}_0) := \inf\{r > 0 \ : \ \operatorname{supp} \mathfrak{v}_0 \subset D(0,r)\}\,. \tag{2}$$

We introduce the *double well* potential

$$V(x) = \mathfrak{v}_0(x - z^\ell) + \mathfrak{v}_0(x - z^r)\,, \qquad (3)$$

where

$$z^\ell = \Big(-\frac{L}{2}, 0\Big), \quad z_r = \Big(\frac{L}{2}, 0\Big)\,. \qquad (4)$$

and

$$L > 2a(\mathfrak{v}_0)\,.$$

The potential wells of V associated with the energy $v_0^{\min}$ are z_ℓ and z_r.

Consider a constant magnetic field $b > 0$, so

$$b = \mathrm{curl}\,(\mathrm{b}\mathbf{A})$$

where $\mathbf{A}$ is defined in polar coordinates (r, θ) as follows,

$$\mathbf{A}(r, \theta) = \frac{r}{2}\begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}. \tag{5}$$

Deep symmetric wells in a strong magnetic field

We consider the Hamiltonian

$$\mathcal{H}_{b,\lambda} := (D - b\mathbf{A})^2 + \lambda^2 V\,, \quad D := \frac{1}{i}\nabla\,, \tag{6}$$

with a double well electric potential $\lambda^2 V$ and a magnetic potential $b\mathbf{A}$. Here, we suppose that $b = \lambda$ and $\lambda \gg 1$ is large.

Regimes where b does not scale like the coupling parameter λ have been considered a long time ago.
For instance, when $b \ll \lambda$, accurate estimates of the tunnel effect where obtained in Helffer-Sjöstrand [HelSjPise1987], while when $b \gg \lambda$, the effect of the potential well becomes weak and the magnetic effect is dominant (see Bellissard [Bel1988] and Helffer-Sjöstrand [HelSjSond1989]).

The potential function considered in (6) is not analytic, thereby making our setting significantly different from the one of [HelSjPise1987]. This will induce difficulties in deriving accurate bounds on the magnitude of the tunnel effect and highlights another interesting new phenomenon related to *tunneling* under a magnetic field compared to recent results:

- by Bonnaillie-Hérau-Raymond [BonHerRay2022] (tunneling inside the boundary Γ for the Neumann realization of the Schrödinger operator with constant magnetic field in an open set Ω)
- by Fournais-Helffer-Kachmar [FoHelKa2022] (tunneling along the discontinuity Γ of a magnetic step).
- see also a recent work (in progress) by Khaled Abou Alfa [AbAl2022] who is considering a case where the magnetic field vanishes along a curve Γ.

Of course, in these questions an assumption of symmetry should be done leading to the existence of symmetric (mini)-wells in Γ.

In order to exploit the connection with semi-classical analysis we consider instead

$$\mathcal{L}_h := (hD - \mathbf{A})^2 + V \,, \tag{7}$$

where $h = \lambda^{-1} \ll 1$.
With $(e_j^{\mathfrak{v}_0}(h))_{j\geq 1}$ the sequence of eigenvalues of $\mathcal{L}_h$, we will investigate the semi-classical asymptotics of

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \,, \tag{8}$$

and prove that, if $\mathfrak{v}_0$ does not vanish in $D\big(0, a\big)$, an asymptotics of the form

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \underset{h\to 0}{=} \exp\left(-\frac{S(\mathfrak{v}_0) + o(1)}{h}\right)$$

Our proof will be based on a mixing between what we get from the semi-classical analysis initiated in Helffer-Sjöstrand and Simon in the eighties with the approach of Fefferman-Shapiro-Weinstein.

Analysis of the Single well operator

Our investigation relies first on expanding the ground state $e^{\mathrm{sw}}(h)$ of the single well Hamiltonian

$$\mathcal{L}_h^{\mathrm{sw}} := (hD - \mathbf{A})^2 + \mathfrak{v}_0 \,, \tag{9}$$

under the additional assumption that $\mathfrak{v}_0$ is radial.

We show that:

Theorem OW: Existence of radial ground states and precise expansions

1. The ground state energy $e^{\mathrm{sw}}(h)$ of $\mathcal{L}_h^{\mathrm{sw}}$, is a simple eigenvalue and
$$e^{\mathrm{sw}}(h) = v_0^{\mathrm{min}} + h\sqrt{1 + 2v_0''(0)} + \mathcal{O}(h^{3/2})\,. \qquad (10)$$

2. There exists a unique positive ground state $\mathfrak{u}_h$, with the properties
   - $\mathfrak{u}_h(x) = u_h(|x|)$ is a radial function ;
   - $\int_{\mathbb{R}^2} |\mathfrak{u}_h(x)|^2 dx = 1$.

Theorem continued

3. There exists a positive radial function $\mathfrak{a}_0$ on $\mathbb{R}^2$ satisfying

$$\mathfrak{a}_0(0) = \frac{1}{2}\frac{\sqrt{1 + 2v_0''(0)}}{\pi}\,, \qquad (11)$$

and s. t. $\forall R > 0$, the ground state $\mathfrak{u}_h$ satisfies, unif. in $B(0, R)$,

$$\left| e^{\mathfrak{d}(x)/h}\mathfrak{u}_h(x) - h^{-1/2}\mathfrak{a}_0(x) \right| = \mathcal{O}(h^{1/2})\,, \qquad (12)$$

where

$$\mathfrak{d}(x) = d(|x|) = \int_0^{|x|} \sqrt{\frac{\rho^2}{4} + v_0(\rho) - v_0^{\min}}\, d\rho\,. \qquad (13)$$

Proof of Theorem OW

Except the "radial" statement, this is rather standard in semi-classical analysis since the works of [HelSj1984] and [Sim1983]. Let us recall the main tools.

The magnetic harmonic approximation

Consider the case where $\mathfrak{v}_0(x) = \mu|x|^2$, where μ is a positive constant. This means that we have replaced $\mathfrak{v}_0$ by its quadratic approximation at 0. The single well operator $\mathcal{L}_h^{sw}$ becomes approximated by

$$\mathcal{L}_h^{\rm swap} = (hD - \mathbf{A})^2 + \mu|x|^2\,.$$

After rescaling[1] we get

$$\sigma(\mathcal{L}_h^{\rm swap}) = h\sigma(L_\mu^{\rm mag})$$

where

$$L_\mu^{\rm mag} = (D - \mathbf{A})^2 + \mu|x|^2\,.$$

[1] We do the change of variable $y = h^{-1/2}x$.

We decompose the operator L_μ^{mag} via the orthogonal projections on the Fourier modes as follows

$$L_\mu^{\mathrm{mag}} \simeq \bigoplus_{m\in\mathbb{Z}} H_{m,\mu}$$

where

$$H_{m,\mu} := \pi_m L_\mu^{\mathrm{mag}} \pi_m^* = -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \left(\frac{1}{4} + \mu\right) r^2 + \frac{m^2}{r^2} - m\,.$$

The min-max principle yields for $m < 0$

$$\lambda_1(H_{m,\mu}) > \inf_{u\neq 0} \frac{\left\langle \left(-\Delta + \left(\frac{1}{4}+\mu\right)|x|^2\right)u, u\right\rangle_{L^2(\mathbb{R}^2)}}{\|u\|_{L^2(\mathbb{R}^2)}} = 2\sqrt{\frac{1}{4}+\mu}\,.$$

Moreover, the rescaling $r \mapsto (1+4\mu)^{1/4} r$ yields the reduction to the unitary equivalent Landau Hamiltonian,

$$\widehat{H}_{m,\mu} = \sqrt{1+4\mu}\, H_{m,0} + \left(\sqrt{1+4\mu} - 1\right) m\,.$$

Consequently, we get

$$\inf_{m\in\mathbb{Z}} \lambda_1(H_m) = \lambda_1(H_0) = \sqrt{1+4\mu}\,, \qquad \inf_{\substack{m\in\mathbb{Z}\\ m\neq 0}} \lambda_1(H_m) > \sqrt{1+4\mu}\,.$$

This implies that

$$\lambda_1(L_\mu^{\mathrm{mag}}) = \sqrt{1+4\mu}$$

is a simple eigenvalue and that its (normalized) associated eigenfunction is radial:

$$\phi_\mu^{\mathrm{mag}}(x) = \pi^{-1/2}(1+4\mu)^{1/4} \exp\left(-\frac{\sqrt{1+4\mu}}{2}|x|^2\right) .$$

Eigenvalue asymptotics and radial ground states

We now have an accurate description of the spectrum of the operator $\mathcal{L}_h^{\mathrm{sw}}$

Proposition

For every fixed $j \in \mathbb{N}$, the j'th eigenvalue of $\mathcal{L}_h^{\mathrm{sw}}$ satisfies,

$$\lambda_j(\mathcal{L}_h^{\mathrm{sw}}) = v_0^{\mathsf{min}} + h\,\lambda_j(L_\mu^{\mathrm{mag}}) + \mathcal{O}(h^{3/2}) \quad (h \to 0_+)\,,$$

with $\mu = \frac{v_0''(0)}{2}$.

Moreover, the lowest eigenvalue of $\mathcal{L}_h^{\mathrm{sw}}$ is simple with a radial ground state.

Agmon estimates

If f is a radial function, then

$$\mathcal{L}_h^{\mathrm{sw}} f = -h^2 \Delta f + \mathfrak{w} f \qquad (14)$$

with

$$\mathfrak{w}(\rho) = \mathfrak{v}_0(\rho) + \frac{1}{4}\rho^2 .$$

Therefore, when restricting the action of $\mathcal{L}_h^{\mathrm{sw}}$ to radial functions, we consider $\mathfrak{w}$ as the effective potential.
Hence, we can apply the semi-classical analysis relative to the Schrödinger operator without magnetic potential as considered in [HelSj1984] or [Sim1983] (see [Hel1988] or [DimSj1999] for a more pedagogical presentation).

Energy identity

The identity above and an integration by parts yield the following result

Proposition

For all $R > 0$, if $\phi \in C^0(\overline{D_R};\mathbb{R})$ and $u \in C^2(\overline{D_R};\mathbb{R})$ are radial functions such that ϕ is Lipschitz and $u = 0$ on ∂D_R, then

$$\int_{D_R} \left(h^2|\nabla(e^{\phi/h}u)|^2 + (\mathfrak{w} - |\nabla\phi|^2|e^{\phi/h}u|^2\right) dx = \int_{D_R} e^{2\phi/h} u\, \mathcal{L}_h^{\mathrm{sw}} u\, dx\,.$$

Application to the decay

We have the following standard application of this proposition on the decay.

Proposition D

For all $\delta \in (0,1)$, there exist $a(\delta), C_\delta, h_0 > 0$ such that $\lim_{\delta \to 0_+} a(\delta) = 0$ and, if $\mathfrak{u}_h$ is a ground state of $\mathcal{L}_h^{\mathrm{sw}}$ and $h \in (0, h_0]$, then we have,

$$\left\| \nabla \left(e^{(1-\delta)\mathfrak{d}(x)/h} \mathfrak{u}_h \right) \right\|^2 + \left\| e^{(1-\delta)\mathfrak{d}(x)/h} \mathfrak{u}_h \right\|^2 \leq C_\delta \, e^{a(\delta)/h} \, \|\mathfrak{u}_h\|^2 \,,$$

where $\mathfrak{d}$ is the Agmon distance associated with $\mathfrak{w} - v_0^{min}$.

WKB approximation

For all $S > 0$, we introduce the set $B_{\mathfrak{d}}(S) = \{x \in \mathbb{R}^2 \ : \ \mathfrak{d}(x) < S\}$, where $\mathfrak{d}$ is the Agmon distance to 0. We can then perform the WKB construction:

Proposition WKB1

There exist $N_0 \geq 1$ and two sequences $(E_k)_{k\geq 0} \subset \mathbb{R}$ and $(\mathfrak{a}_k)_{k\geq 0} \subset C^\infty(\mathbb{R}^2)$ s. t. , for all $N \geq 1$ and $S > 0$,

$$e^{\mathfrak{d}(x)/h}\Big(\mathcal{L}_h^{\mathrm{sw}} - E^N(h)\Big)\vartheta^N = \mathcal{O}(h^{N-N_0}) \quad \text{on } B_{\mathfrak{d}}(S)\,,$$

where

$$E^N(h) = \sum_{k=0}^{N} E_k h^k\,, \quad E_0 = v_0^{\min}, \quad E_1 = \sqrt{1 + 2v_0''(0)}$$

$$\vartheta^N(x) = h^{-1/2}\left(\sum_{k=0}^{N} \mathfrak{a}_k(x) h^k\right) e^{-\mathfrak{d}(x)/h}, \quad \mathfrak{a}_0(0) = \frac{1}{2}\sqrt{\frac{1+2v_0''(0)}{\pi}}\,.$$

The function $\mathfrak{a}_0$ satisfies the transport equation

$$2\nabla\mathfrak{d}\cdot\nabla\mathfrak{a}_0+(\Delta\mathfrak{d}-E_1)\mathfrak{a}_0=0\,.$$

Since $\mathfrak{d}$ and $\mathfrak{a}_0$ are radial, we get

$$\mathfrak{a}_0(x)=a_0(|x|):=\frac{1}{2}\sqrt{\frac{1+2v_0''(0)}{\pi}}\exp\left(-\int_0^{|x|}f(\rho)d\rho\right)\,,$$

where

$$f(\rho)=\frac{1}{4}\frac{u'(\rho)}{u(\rho)}+\frac{1}{2\rho}-\frac{E_1}{2\sqrt{u(\rho)}}\,,$$

and

$$u(\rho)=\frac{\rho^2}{4}+v_0(\rho)-v_0^{\min}\,.$$

Proposition WKB2

There exists $N_0 \geq 1$, and for all $h \in (0, h_0]$, there exists a normalized ground state $\mathfrak{u}_h$ of $\mathcal{L}_h^{\mathrm{sw}}$ s. t. for any N and any $R > 0$ the following holds

$$\left\| e^{\mathfrak{d}(x)/h}(\mathfrak{u}_h - \vartheta^N) \right\|_{H^2(D(0,R))} = \mathcal{O}(h^{N-N_0}) \,.$$

This ends the sketch of the proof of Theorem OW.

Coming back to the main theorem

Our "one well" theorem OW in particular clarifies the hypotheses imposed in Fefferman-Shapiro-Weinstein which states then that when

$$\mathfrak{v}_0 \leq 0 \text{ and } L > 4\left(\sqrt{|v_0^{\min}|} + a(\mathfrak{v}_0)\right) , \qquad (15)$$

then

$$\exp\left(-\frac{L^2 + 4\sqrt{|v_0^{\min}|}L + \gamma(\mathfrak{v}_0)}{4h}\right) \leq e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \qquad (16)$$

where $\gamma(\mathfrak{v}_0)$ is a positive constant, and

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \leq Ch^{-5/2}\exp\left(-\frac{(L - a(\mathfrak{v}_0))^2 - a(\mathfrak{v}_0)^2}{4h}\right) . \qquad (17)$$

The most important was here to give a lower bound but we will see that these estimates are far from optimal.

Interaction matrix or hopping coefficient

The bounds above follow from the asymptotics [FeShWe2022]

$$e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h) \underset{h\to 0}{\sim} \left| 2 \int_{D(0,a)} \mathfrak{v}_0(x)\mathfrak{u}_h(x)\mathfrak{u}_h(x_1 + L, x_2) e^{\frac{iLx_2}{2h}} \, dx \right| \tag{18}$$

where $\mathfrak{u}_h$ is the radial ground state of $\mathcal{L}_h^{\mathrm{sw}}$.
The integral in the right hand side is called in Solid State Physics the *hopping coefficient.* Under different conditions, it can be derived through a reduction to the restriction of $\mathcal{L}_h$ on a two dimensional space, yielding an *interaction matrix* like in [Hel1988] or [DimSj1999]. The hopping parameter corresponds with the off diagonal term in the 2×2 interaction matrix.

Using the improved expansion of the ground state $\mathfrak{u}_h$, we improve the bounds on the hopping coefficient and thereby on $e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h)$ provided $\mathfrak{v}_0$ satisfies the conditions in (1).

Besides its role in capturing the tunneling asymptotics, precise estimates of the hopping coefficient (or the so-called interaction matrix) are key ingredients in the understanding of tight binding reductions in Solid State Physics (see [ShWe2022] and earlier [Out1987, Dau1994, DimSj1999] for mathematical contributions).

Our main result, on the eigenvalue splitting, is

[HK]-Theorem: Sharp asymptotics of the eigenvalue splitting

Under the previous assumptions, if $\mathfrak{v}_0 < 0$ in $D\big(0, a)\big)$, then we have

$$h \ln\left(e_2^{\mathfrak{v}_0}(h) - e_1^{\mathfrak{v}_0}(h)\right) \underset{h \to 0}{\sim} -S(\mathfrak{v}_0)\,,$$

where $S(\mathfrak{v}_0)$ is a positive explicit constant.

The formula for $S(\mathfrak{v}_0)$

$$S(\mathfrak{v}_0) = -F(\mathfrak{v}_0) + \inf_{\substack{r\in[0,a]\\ t\in(0,+\infty)}} \Psi(r,t)\,,$$

where

$$\Psi(r,t) := d(r) + \frac{r^2+L^2}{4}(2t+1) + \frac{|v_0^{\min}|}{2}\ln\left(1+\frac{1}{t}\right) - Lr\sqrt{t(t+1)} \tag{19}$$

and

$$F(\mathfrak{v}_0) = \frac{a}{4}\sqrt{a^2+4|v_0^{\min}|} + |v_0^{\min}|\ln\frac{\left(\sqrt{a^2+4|v_0^{\min}|}+a\right)^2}{4|v_0^{\min}|} - d(a) \tag{20}$$

Analyzing the infimum of Ψ

If $L > 2a$, then

$$\min_{(r,t)\in[0,a]\times\mathbb{R}_+} \Psi(r,t) = \Psi(a, t_a)\,,$$

where

$$t_a = \sqrt{\frac{1}{4} + s_+(a, L, v_0^{\min})} - \frac{1}{2}$$

and

$$s_+(a, L, v_0^{\min}) := \frac{2|v_0^{\min}|(L^2 + a^2) + L^2 a^2}{2(L^2 - a^2)^2} + \frac{1}{L^2 - a^2}\sqrt{\frac{(2|v_0^{\min}|(L^2 + a^2) + L^2 a^2)^2}{4(L^2 - a^2)^2} - |v_0^{\min}|^2}\,.$$

Moreover, (a, t_a) is the unique minimum of Ψ.

An important representation formula

Representation formula

The radial ground state $\mathfrak{u}_h$ has the following representation for $\rho \geq a$,

$$u_h(\rho) = C_h \exp\left(-\frac{\rho^2}{4h}\right) \int_0^{+\infty} \exp\left(-\frac{\rho^2 t}{2h}\right) t^{\alpha-1}(1+t)^{-\alpha} dt \,,$$

where

$$\alpha = \frac{1}{2h}|v_0^{\min}| - \frac{1}{2}\left(\sqrt{1+2v_0''(0)} - 1\right) + \mathcal{O}(h^{1/2}) \underset{h\to 0}{\sim} \frac{1}{2h}|v_0^{\min}| \,,$$

and

$$C_h \underset{h\to 0}{\sim} C_h^{\mathrm{asy}} := \mathfrak{m}(v_0)h^{-1}\exp\left(\frac{F(\mathfrak{v}_0)}{h}\right) .$$

Here $a = a(\mathfrak{v}_0)$ and

$$F(\mathfrak{v}_0) = \frac{a}{4}\sqrt{a^2 + 4|v_0^{\min}|} + |v_0^{\min}| \ln \frac{\left(\sqrt{a^2 + 4|v_0^{\min}|} + a\right)^2}{4|v_0^{\min}|} - d(a)$$

$$m(\mathfrak{v}_0) = \frac{\mathfrak{a}_0(0)}{4|v_0^{\min}|\sqrt{2\pi a}} \left(a^2 + 4|v_0^{\min}|\right)^{1/4} \left(\sqrt{a^2 + 4|v_0^{\min}|} + a\right)^2 .$$

$$\alpha = \frac{1}{2} - \frac{1}{2h} e^{\mathrm{sw}}(h) .$$

Second representation formula

We start by expressing the hopping coefficient in polar coordinates

$$w_{\ell,r} = \int_0^a r\, v_0(r) u_h(r) \left(\int_0^{2\pi} K_h(r,\theta) d\theta \right) dr\,, \tag{21}$$

where

$$K_h(r,\theta) := u_h(r^2 + L^2 + 2Lr\cos\theta) e^{\frac{iLr\sin\theta}{h}}\,.$$

The integral of K_h with respect to θ is computed in [FeShWe2022, Prop. 5.1] as follows

$$\int_0^{2\pi} K_h(r,\theta)d\theta = C_h \exp\left(-\frac{r^2+L^2}{4h}\right)\int_0^{+\infty} G_h(r,t)dt\,, \qquad (22)$$

where

$$G_h(r,t) = \exp\left(-\frac{(r^2+L^2)t}{2h}\right) t^{\alpha-1}(1+t)^{-\alpha} I_0\left(\frac{Lr\sqrt{t(t+1)}}{h}\right) \qquad (23)$$

and

$$z \mapsto I_0(z) = \frac{1}{2\pi}\int_0^{\pi} e^{z\cos\theta} d\theta\,.$$

The advantage of the second representation formula is the absence of the oscillatory complex term and moreover, the integrand G_h is a positive function. The function $I_0(z)$ has the following asymptotic for large $z > 0$,

$$I_0(z) \underset{z \to +\infty}{\sim} \frac{e^z}{\sqrt{2\pi z}} \,.$$

In addition we have the universal upper bound

$$I_0(z) \leq e^z \,.$$

Merci. Thanks.

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