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On the ground state energy for a magnetic Schrödinger operator and the effect of the de Gennes boundary condition

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Abstract

Motivated by the Ginzburg–Landau theory of superconductivity, we estimate the ground state energy of a magnetic Schrödinger operator with de Gennes boundary condition in the semi-classical limit and we study the localization of the corresponding ground states. We exhibit cases when the de Gennes boundary condition has a strong effect on this localization. **To cite this article:** A. Kachmar, *C. R. Acad. Sci. Paris, Ser. I 342 (2006)*.

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Résumé

Sur l'énergie de l'état fondamental d'un opérateur de Schrödinger avec un champ magnétique et l'effet de la condition au bord de de Gennes. Motivé par la théorie de Ginzburg–Landau de supraconductivité, nous estimons dans le régime semi-classique l'énergie de l'état fondamental d'un opérateur de Schrödinger avec champ magnétique et condition au bord de de Gennes. Nous obtenons des cas où la condition au bord de de Gennes a un effet fort sur cette localisation. **Pour citer cet article :** A. Kachmar, *C. R. Acad. Sci. Paris, Ser. I 342 (2006)*.

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Comme le physicien de Gennes l'explique dans [3], le comportement de la supraconductivité dans un matériau cylindrique de section $\Omega \subset \mathbb{R}^2$ entouré par un autre matériau est décrit par les minimiseurs de la fonctionnelle de Ginzburg–Landau :

$$\mathcal{G}(\phi, \mathcal{A}) = \int_{\Omega} \left\{ |\nabla - i\sigma\kappa\mathcal{A}\phi|^2 + \sigma^2\kappa^2 |\operatorname{curl} \mathcal{A} - 1|^2 + \frac{\kappa^2}{2} (|\phi|^2 - 1)^2 \right\} dx + \int_{\partial\Omega} \tilde{\gamma}(x; \kappa) |\phi(x)|^2 dx, \quad (1)$$

définie pour $(\phi, \mathcal{A}) \in H^1(\Omega; \mathbb{C}) \times H^1(\Omega; \mathbb{R}^2)$. Le paramètre σ est l'intensité du champ magnétique appliqué, κ est une caractéristique du matériau et $\tilde{\gamma}(\cdot; \kappa)$ est une fonction C^∞ sur le bord (appelée dans la littérature physique et

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dans le cas où elle est constante paramètre de de Gennes). Pour un minimiseur global (ψ, A) de (1), la fonction ψ est appelée le paramètre d'ordre et son amplitude rend compte de la densité des paires de Cooper dans Ω . Le champ de vecteur A est appelé le potentiel magnétique induit. La fonction ψ satisfait alors la condition au bord dite de de Gennes : $\nu \cdot (\nabla - i\sigma\kappa A)\psi + \tilde{\gamma}(x; \kappa)\psi = 0$, où ν est le vecteur normal unité extérieur de $\partial\Omega$. Dans d'autres contextes, cette condition est appelée Condition de Robin.

L'équation d'Euler–Lagrange associée à la fonctionnelle \mathcal{G} admet une solution $(0, A)$, appelée solution normale, telle que $\text{rot } A = 1$. Il est alors naturel d'étudier si cette paire est un minimum local de la fonctionnelle \mathcal{G} , ce qui conduit immédiatement à l'étude de la positivité de la forme quadratique :

$$H^1(\Omega) \ni \phi \mapsto \mathcal{Q}_{\sigma\kappa A, \tilde{\gamma}, \Omega}(\phi) = (\sigma\kappa)^2 q_{h,A,\Omega}^{\alpha,\gamma}(\phi) - \kappa^2 \|\phi\|_{L^2(\Omega)}^2,$$

où $h = \frac{1}{\sigma\kappa}$, $\tilde{\gamma}(x; \kappa) = h^{\alpha-1}\gamma(x)$, et

$$q_{h,A,\Omega}^{\alpha,\gamma}(\phi) = \|(h\nabla - iA)\phi\|_{L^2(\Omega)}^2 + h^{1+\alpha} \int_{\partial\Omega} \gamma(x)|\phi|^2 dx. \quad (2)$$

Le paramètre $\alpha > 0$ est introduit dans le but de contrôler la taille de la fonction $\tilde{\gamma}(\cdot; \kappa)$. Nous noterons :

$$\mu^{(1)}(\alpha, \gamma, h) = \inf\{q_{h,A,\Omega}^{\alpha,\gamma}(u); u \in H^1(\Omega); \|u\|_{L^2(\Omega)} = 1\}.$$

Nous sommes intéressés à estimer $\mu^{(1)}(\alpha, \gamma, h)$ dans le régime semi-classique $h \rightarrow 0$. Nous établissons un développement limité de premier ordre de $\mu^{(1)}(\alpha, \gamma, h)$ dans le Théorème 3.1. Ce développement dépend fortement de α . En particulier, si $\alpha \geq \frac{1}{2}$, nous avons un comportement semblable à celui de Neumann ($\gamma = 0$). Si $\alpha \in]0, \frac{1}{2}[$ et $\gamma_0 > 0$, nous avons un comportement semblable à celui de la réalisation de Dirichlet. Si $\alpha \in]0, \frac{1}{2}[$ et $\gamma_0 < 0$, $\frac{\mu^{(1)}(\alpha, \gamma, h)}{h}$ est négatif et tend vers $-\infty$ lorsque $h \rightarrow 0$.

Pour $\alpha \geq \frac{1}{2}$, nous déterminons ensuite des développements limités plus fins dans les Théorèmes 4.1 et 4.2, qui montrent l'effet de la courbure scalaire κ_r et de la fonction γ . Le cas $\alpha = 1$ est particulier dans le sens où γ et κ_r ont le même ordre dans le développement limité de $\mu^{(1)}(\alpha, \gamma, h)$.

Cette étude complète celle de Lu–Pan [11] et c'est une première étape dans l'analyse de l'apparition de la supra-conductivité dans le même esprit que les travaux de Lu–Pan [10,11] et Helffer–Pan [8].

1. Introduction

Let us consider an open bounded set $\Omega \subset \mathbb{R}^2$ with regular boundary. For a vector field $A \in C^\infty(\overline{\Omega}; \mathbb{R}^2)$ such that $\text{curl } A = 1$, a regular real valued function $\gamma \in C^\infty(\partial\Omega; \mathbb{R})$ and a number $\alpha > 0$, let us consider the self-adjoint magnetic Schrödinger operator $P_{h,A,\Omega}^{\alpha,\gamma}$ defined by:

$$D(P_{h,A,\Omega}^{\alpha,\gamma}) = \{u \in H^2(\Omega); \nu \cdot (h\nabla - iA)u|_{\partial\Omega} + h^\alpha \gamma u|_{\partial\Omega} = 0\}, \quad P_{h,A,\Omega}^{\alpha,\gamma} = -(h\nabla - iA)^2. \quad (3)$$

The parameter h is called the semi-classical parameter. We denote by $\mu^{(1)}(\alpha, \gamma, h)$ the ground state energy (or lowest eigenvalue) of $P_{h,A,\Omega}^{\alpha,\gamma}$. Our aim is to estimate $\mu^{(1)}(\alpha, \gamma, h)$ as h tends to 0.

As in [7,11], a first step is to understand the model case of the half-plane when the function γ and the magnetic field are both constant.

2. The model operator

Let us consider the magnetic potential $A_0(x_1, x_2) = (-x_2, 0)$, $\forall (x_1, x_2) \in \mathbb{R} \times \mathbb{R}_+$. For $\gamma \in \mathbb{R}$, we define the self-adjoint operator $P[\gamma] = -(\nabla - iA_0)^2$ on the domain:

$$D(P[\gamma]) = \{u \in L^2(\mathbb{R} \times \mathbb{R}_+); (\nabla - iA_0)u, (\nabla - iA_0)^2 u \in L^2(\mathbb{R} \times \mathbb{R}_+), \partial_{x_2} u = \gamma u \text{ at } x_2 = 0\}.$$

We denote by $\Theta(\gamma)$ the bottom of the spectrum of $P[\gamma]$. Actually, we are interested in the bottom of the spectrum of the operator $P_{h,A_0,\mathbb{R} \times \mathbb{R}_+}^{\alpha,\gamma}$, but a scaling argument gives

$$\forall h \in \mathbb{R}_+, \forall \alpha, \gamma \in \mathbb{R}, \quad \inf \text{Sp}(P_{h,A_0,\mathbb{R} \times \mathbb{R}_+}^{\alpha,\gamma}) = h\Theta(h^{\alpha-1/2}\gamma).$$

By a partial Fourier transformation with respect to the first variable, we get the ξ -family of one-dimensional operators:

$$H[\gamma, \xi] = -\frac{d^2}{dt^2} + (t - \xi)^2, \tag{4}$$

with domain

$$D(H[\gamma, \xi]) = \{u \in H^2(\mathbb{R}_+); (t - \xi)^j u \in L^2(\mathbb{R}_+), j = 1, 2; u'(0) = \gamma u(0)\}. \tag{5}$$

Note that the operator $H[\gamma, \xi]$ has compact resolvent. We denote by $\mu^{(1)}(\gamma, \xi)$ the first eigenvalue (necessarily simple) of $H[\gamma, \xi]$. A spectral analysis using the separation of variables (cf. [13]) permits to show that:

$$\Theta(\gamma) = \inf_{\xi \in \mathbb{R}} \mu^{(1)}(\gamma, \xi). \tag{6}$$

Following the method of Dauge–Helffer [4], we get that for each $\gamma \in \mathbb{R}$, $\Theta(\gamma) < 1$ and that the function $\xi \mapsto \mu^{(1)}(\gamma, \xi)$ attains its minimum at a unique point $\xi(\gamma) > 0$ satisfying

$$\xi(\gamma)^2 = \Theta(\gamma) + \gamma^2. \tag{7}$$

We denote by φ_γ the unique strictly positive and L^2 -normalized eigenfunction associated to the eigenvalue $\Theta(\gamma)$. We get now that the function:

$$\phi_\gamma(x_1, x_2) = \exp(-i\xi(\gamma)x_1)\varphi_\gamma(x_2) \tag{8}$$

satisfies $P[\gamma]\phi_\gamma = \Theta(\gamma)\phi_\gamma$ and hence it behaves like an eigenfunction for the operator $P[\gamma]$.

A modification of Grushin’s method [6] permits to show that the functions $\Theta(\gamma)$ and $\gamma \mapsto \varphi_\gamma \in L^2(\mathbb{R}_+)$ are C^∞ on \mathbb{R} (cf. [9]).

By using the function $e^{\gamma t} \varphi_0$ as a trial function for the operator $H[\gamma, \xi(\gamma)]$, we get by the spectral theorem:

$$\Theta'(\gamma) = |\varphi_0(0)|^2. \tag{9}$$

The analysis of the Neumann problem in [2] gives the following decay when γ is sufficiently large:

$$1 - C_0\gamma \exp -\gamma^2 \leq \Theta(\gamma) < 1, \quad \forall \gamma \in [\gamma_0, +\infty[. \tag{10}$$

We have the following decay when $\gamma < 0$:

$$-\gamma^2 \leq \Theta(\gamma) \leq -\gamma^2 + \frac{1}{4\gamma^2}, \quad \forall \gamma \in]-\infty, 0[. \tag{11}$$

Note that the lower bound given above is a direct consequence of the relation (7). For the upper bound, we use the function $e^{\gamma t}$ (with $\gamma < 0$) as a trial function for the quadratic form defining $H[\gamma, 0]$.

3. Asymptotics

Having analyzed in detail the model operator, we come back to the general situation and give an asymptotics for $\mu^{(1)}(\alpha, \gamma, h)$ as h tends to 0. Let $\gamma_0 = \min_{x \in \partial\Omega} \gamma(x)$. From the expression of the quadratic form in (2), when looking for a lower bound of $\mu^{(1)}(\alpha, \gamma, h)$, it is natural to start by finding a lower bound of $\mu^{(1)}(\alpha, \gamma_0, h)$. Using the technique of [7], we use a fine partition of unity of \mathbb{R}^2 where the size of the partition’s support is of order $h^{3/8}$. The main contribution is then due to terms where the partition’s support meets the boundary. After a change of variables, we compare with the model operator in the half-plane. In this way we get positive constants C, C' and h_0 such that:

$$\mu^{(1)}(\alpha, \gamma, h) \geq h\Theta(h^{\alpha-1/2}\gamma_0(1 + C'h^{1/4})) - Ch^{5/4}, \quad \forall h \in]0, h_0[. \tag{12}$$

When looking for an upper bound of $\mu^{(1)}(\alpha, \gamma, h)$, it is a natural idea to construct a trial function supported near a point x_0 of the boundary where γ is minimum so that we can approximate γ by γ_0 modulo a small error. In a tubular neighborhood of $\partial\Omega$, let us consider the coordinates (s, t) where t measures the distance to $\partial\Omega$ and s measures the distance in $\partial\Omega$. We suppose that $x_0 = 0$ in the (s, t) coordinates and we define the following trial function supported near x_0 :

$$u_{h,\alpha} = a^{-1/2}h^{-3/8}\chi(t) \times f(h^{-1/4}s)\phi_\eta(h^{-1/2}s, h^{-1/2}t), \tag{13}$$

where $a(s, t) = 1 - t\kappa_r(s)$, κ_r is the scalar curvature, the function χ is a cut-off equal to 1 in a compact interval $[0, \frac{\eta_0}{2}]$ and the function $f \in C_0^\infty(]-\frac{1}{2}, \frac{1}{2}[; \mathbb{R})$ is chosen such that $\|f\|_{L^2(\mathbb{R})} = 1$. The function ϕ_η defined in (8) is the eigenfunction for the model operator and $\eta = h^{\alpha-1/2}(\gamma_0 + Ch^{1/2})$ where C is an appropriate positive constant. By computing $q_{h,A,\Omega}^{\alpha,\gamma}(u_{h,\alpha})$, we get the following upper bound:

$$\mu^{(1)}(\alpha, \gamma, h) \leq h\Theta(h^{\alpha-1/2}(\gamma_0 + Ch^{1/2})) + \tilde{C}h^{3/2}, \quad \forall h \in]0, h_0]. \tag{14}$$

Remark 1. When $\alpha \in]\frac{1}{2}, 1[$, we get from (14) and (9) the following upper bound,

$$\mu^{(1)}(\alpha, \gamma, h) \leq h\Theta(0) + 3C_1\gamma_0h^{\alpha+1/2} + \mathcal{O}(h^{\inf(3/2, 2\alpha)}),$$

where $C_1 := \frac{|\varphi_0(0)|^2}{3}$. This upper bound is actually an asymptotic expansion of $\mu^{(1)}(\alpha, \gamma, h)$.

Using (9), (10) and (11), we get from (12) and (14) the following theorem.

Theorem 3.1. *The ground state energy of the operator $P_{h,A,\Omega}^{\alpha,\gamma}$ satisfies as h tends to 0:*

$$\mu^{(1)}(\alpha, \gamma, h) \sim h\Theta(h^{\alpha-1/2}\gamma_0). \tag{15}$$

The asymptotics (15) depends strongly on α and γ_0 does not always appear effectively. However, if $\gamma_0 \leq 0$ or $\frac{1}{2} \leq \alpha < 1$, then $\lim_{h \rightarrow 0} \frac{\mu^{(1)}(\alpha, \gamma, h)}{h} < 1$ and a ground state is localized as $h \rightarrow 0$ near the boundary points where the function γ is minimum.

4. Curvature effects

In the case when $\alpha \geq \frac{1}{2}$, we give a two terms asymptotics for $\mu^{(1)}(\alpha, \gamma, h)$.

Theorem 4.1. *Suppose that $\alpha = 1$. Then the ground state energy of the operator $P_{h,A,\Omega}^{1,\gamma}$ satisfies as h tends to 0:*

$$\mu^{(1)}(1, \gamma, h) = h\Theta(0) - C_1(\kappa_r - 3\gamma)_{\max}h^{3/2} + \mathcal{O}(h^{13/8}). \tag{16}$$

Moreover the ground states are localized near the boundary points where $\kappa_r - 3\gamma$ is maximum.

If γ is constant, the remainder in (16) is better and of order $\mathcal{O}(h^{5/3})$. We have recovered in the above theorem the result of [7] which deals with the case $\gamma = 0$.

Theorem 4.2. *Suppose that $\alpha \geq \frac{1}{2}$ and γ is constant, then the ground state energy of the operator $P_{h,A,\Omega}^{\alpha,\gamma}$ satisfies as h tends to 0:*

$$\mu^{(1)}(\alpha, \gamma, h) = h\Theta(h^{\alpha-1/2}\gamma) - C_1(\alpha, \gamma)(\kappa_r)_{\max}h^{3/2} + o(h^{3/2}), \tag{17}$$

where $C_1(\alpha, \gamma) = \frac{|\varphi_0(0)|^2}{3}$ if $\alpha > \frac{1}{2}$ and $C_1(\frac{1}{2}, \gamma) = \frac{1}{6}[1 + (\gamma\xi(\gamma))^2]|\varphi_\gamma(0)|^2$ if $\alpha = \frac{1}{2}$.

To prove the above two theorems, we have to introduce a ‘refined’ family of model operators. For $\eta, \beta \in \mathbb{R}$ and $\delta \in]\frac{1}{4}, \frac{1}{2}[$, let us consider the one-dimensional ξ -family of self-adjoint operators on the space $L^2(]0, h^{\delta-1/2}[; (1 - h^{1/2}\beta t) dt)$:

$$H_{h,\beta,\xi}^{\alpha,\eta,D} = -\partial_t^2 + (t - \xi)^2 + \beta h^{1/2}(1 - \beta h^{1/2}t)^{-1}\partial_t + 2\beta h^{1/2}t \left(t - \xi - \beta h^{1/2}\frac{t^2}{2} \right)^2 - \beta h^{1/2}t^2(t - \xi) + \beta^2 h \frac{t^4}{4},$$

with domain:

$$D(H_{h,\beta,\xi}^{\alpha,\eta,D}) = \{u \in H^2(]0, h^{\delta-1/2}[; u'(0) = h^{\alpha-1/2}\eta u(0), u(h^{\delta-1/2}) = 0\}.$$

We have then to find (when $\eta, \beta \in]-M, M[$ and M a given positive constant), uniformly with respect to $\xi \in \mathbb{R}$, a lower bound for the first eigenvalue $\mu_1(H_{h,\beta,\xi}^{\alpha,\eta,D})$ of the operator $H_{h,\beta,\xi}^{\alpha,\eta,D}$. Because we are interested in $\inf_{\xi \in \mathbb{R}} \mu_1(H_{h,\beta,\xi}^{\alpha,\eta,D})$, it is sufficient to consider ξ 's satisfying $|\xi - \xi(\tilde{\eta})| \leq \zeta h^\rho$, where ζ, ρ are positive constants independent of h and $\tilde{\eta} = h^{\alpha-1/2}\eta$. We look for a formal solution $(\mu, f_{h,\beta,\xi}^{\alpha,\eta})$ to

$$H_{h,\beta,\xi}^{\alpha,\eta} f_{h,\beta,\xi}^{\alpha,\eta} = \mu f_{h,\beta,\xi}^{\alpha,\eta}, \quad (f_{h,\beta,\xi}^{\alpha,\eta})'(0) = h^{\alpha-1/2}\eta f_{h,\beta,\xi}^{\alpha,\eta}(0), \quad \text{in } \mathbb{R}_+, \tag{18}$$

in the form:

$$\mu = d_0 + d_1(\xi - \xi(\tilde{\eta})) + d_2(\xi - \xi(\tilde{\eta}))^2 + d_3 h^{1/2}, \quad f_{h,\beta,\xi}^{\alpha,\eta} = u_0 + (\xi - \xi(\tilde{\eta}))u_1 + (\xi - \xi(\tilde{\eta}))^2 u_2 + h^{1/2}u_3.$$

The coefficients d_0, d_1, d_2, d_3 and the functions u_0, u_1 are given by:

$$d_0 = \Theta(\tilde{\eta}), \quad d_1 = 0, \quad d_2 = 1 - 2 \int_{\mathbb{R}_+} (t - \xi(\tilde{\eta}))\varphi_{\tilde{\eta}} u_1 dt, \quad d_3 = \beta \int_{\mathbb{R}_+} \varphi_{\tilde{\eta}} \{ \partial_t + (t - \xi(\tilde{\eta}))^3 \} \varphi_{\tilde{\eta}} dt,$$

$$u_0 = \varphi_{\tilde{\eta}}, \quad u_1 = 2(-\partial_t^2 + (t - \xi(\tilde{\eta}))^2 - \Theta(\tilde{\eta}))^{-1} \{ (t - \xi(\tilde{\eta}))\varphi_{\tilde{\eta}} \}.$$

By standard Fredholm theory, the operator $(-\partial_t^2 + (t - \xi(\tilde{\eta}))^2 - \Theta(\tilde{\eta}))^{-1}$ is defined on the orthogonal space of $\varphi_{\tilde{\eta}}$ and has values in $D(H[\tilde{\eta}, \xi(\tilde{\eta})])$ (cf. (5)).

Note that, using Agmon's technique (cf. [1]), the function $f_{h,\beta,\xi}^{\alpha,\eta}$ decays exponentially at infinity and we can control its decay uniformly with respect to h . Then by using the function $\chi(\frac{t}{h^{\delta-1/2}})f_{h,\beta,\xi}^{\alpha,\eta}$ (where χ is the same as in (13)) as a quasi-mode for the operator $H_{h,\beta,\xi}^{\alpha,\eta,D}$, we get by the spectral theorem,

$$|\mu_1(H_{h,\beta,\xi}^{\alpha,\eta,D}) - \{ \Theta(\tilde{\eta}) + d_2(\xi - \xi(\tilde{\eta}))^2 + d_3 h^{1/2} \}| \leq C[h^{1/2}|\xi - \xi(\tilde{\eta})| + h^{\delta+1/2}].$$

We show that $d_2 > 0$ and if $\alpha > \frac{1}{2}$, $d_3 = \frac{|\varphi_0(0)|^2}{3}$ modulo $\mathcal{O}(h^{\alpha-1/2})$. If $\alpha = \frac{1}{2}$, we show that $d_3 = C_1(\alpha, \eta)$. This permits (cf. [9]) to obtain a lower bound for $\mu^{(1)}(\alpha, \gamma, h)$.

5. Conclusion

We have extended in Theorems 4.1 and 4.2 the two term expansion announced by Pan [12] in the particular case when $\alpha = 1$ and γ is a positive constant. The systematic analysis in the spirit of [7] had allowed us to understand the role of the boundary condition imposed by de Gennes. We have found a specific difficulty when γ is negative. Note that negative values of γ were considered in the physical literature [5]. We have not been able to obtain the localization of the ground state when $\alpha < 1/2$ and $\gamma_0 > 0$. This situation is strongly related to the question of the localization of the ground state of the Dirichlet realization of the Schrödinger operator with constant magnetic field which is an open problem. Finally, in the spirit of [8,11], we hope to apply this analysis to the onset of superconductivity (cf. [9]).

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