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Operator ordering and continuum limit for path integrals: a toy model

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Abstract

We address the problem of continuum limit for path integrals in quantum systems where the operator ordering is ambiguous. A two-dimensional (2d) electron in a harmonic potential in the presence of a perpendicular magnetic field serves as a toy model. We, first, reorder operators in the Hamiltonian following a special "antiordering" procedure to obtain correct continuum limit. We use adiabatic expansion to present a propagator as a path integral for slow variables. We then show that the "antiordering" procedure solves the problem only in the case of projection onto the lowest Landau level.

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The problem of continuum limit for path integral formalism is of a great interest [1–3]. If this limit exists, it must correspond to a particular operator ordering in the Hamiltonian. One can illustrate this problem in the simplest case of an electron in a magnetic field. The correct continuum limit is obtained only if the vector-potential in the phase-space path integral is evaluated in the midpoint of each interval (midpoint rule) which corresponds to a symmetric ordering of coordinate $\mathbf{x}$ and momentum $\hat{\mathbf{p}}$ operators. In general case the orders of integration and the continuum limit cannot be interchanged. This procedure fails for both configuration-space and phase-space path integrals [4]. The coherent-state representation of propagators [5] as well-defined phase-space path integrals on continuous phase-space paths

was proposed [4], including a special "antiordering" procedure. In Appendix we illustrate this method for a one-dimensional (1d) quantum oscillator.

Present work was motivated by the idea of adiabatic expansion proposed in [6]. This paper considers an electron in a 2d plane and a perpendicular magnetic field in the presence of an arbitrary potential $V(x, y)$. After the standard change of variables in the magnetic field B

$$\hat{\boldsymbol{\pi}} = \hat{\mathbf{p}} - \frac{e\mathbf{A}}{c},\ \hat{X} = x - \frac{c\hat{\pi}_y}{eB},\ \hat{Y} = y + \frac{c\hat{\pi}_x}{eB}, \tag{1}$$

where introduced operators have the following commutation relations:

$$[\hat{X}, \hat{Y}] = \frac{ic}{eB},\ [\hat{\pi}_x, \hat{\pi}_y] = \frac{ieB}{c},\ [\hat{X}, \hat{\pi}_{x,y}] = [\hat{Y}, \hat{\pi}_{x,y}] = 0. \tag{2}$$

(operators X and Y are called guiding center coordinates) the Hamiltonian is then presented as

$$\hat{H} = \frac{\hat{\pi}_x^2}{2m} + \frac{\hat{\pi}_y^2}{2m} + V(\hat{X} + \frac{c\hat{\pi}_y}{eB}, \hat{Y} - \frac{c\hat{\pi}_x}{eB}). \tag{3}$$

The idea of adiabatic expansion [6] is to treat slow variables $X(t)$ and $Y(t)$ as functions of time, while keeping $\hat{\pi}_x$ and $\hat{\pi}_y$ as operators in the path integral. Then it is possible to write down a Schrödinger equation for the fast variable π_y considering X and Y as fixed parameters. Using solutions of this equation in the adiabatic basis (wavefunctions $\psi_n(\pi_y, X, Y)$ and eigenenergies $\epsilon_n(X, Y)$) one finally obtains a propagator for $X(t)$ and $Y(t)$ with an effective action S, which can be treated semiclassically.

$$S = \int_{t_i}^{t_f} \left[\frac{eB}{2c}(Y\dot{X} - X\dot{Y}) + f_n(X,Y)\dot{X} + g_n(X,Y)\dot{Y} - \epsilon_n(X,Y) \right] dt, \tag{4}$$

where $f_n(X,Y) = i\langle\psi_n \mid \frac{\partial}{\partial X} \mid \psi_n\rangle$, $g_n = i\langle\psi_n \mid \frac{\partial}{\partial Y} \mid \psi_n\rangle$ (we put $\hbar \equiv 1$ through the rest of the paper). The sum of the second and third terms represent the Berry phase as was mentioned in [6]. This effective action allows to calculate eigenvalues of energy using semiclassical quantization condition [6–8]. It can further serve as the starting point in the investigation of the floating of extended states at low magnetic fields in quantum Hall systems [9–12]. Tunneling in the presence of a perpendicular magnetic field can be studied as well. The formalism of [6] uses arbitrary operator ordering, but according to [4, 5], a phase-space path integral formalism cannot define the correct continuum limit. In order to check whether the procedure proposed in [4] would allow to avoid this ambiguity and improve the accuracy of the

results we consider below a toy model: an electron in a 2d harmonic potential in the presence of a perpendicular magnetic field.

First, we describe briefly the "antiordering" procedure, proposed in [4]. Starting with the Hamiltonian $H(p,q)$, one defines annihilation and creation operators

$$\hat{a} = \frac{1}{\sqrt{2}}\left(q + i\hat{p})\right),\ \hat{a}^\dagger = \frac{1}{\sqrt{2}}\left(q - i\hat{p})\right), \tag{5}$$

and then using commutation relation $[\hat{a}, \hat{a}^\dagger] \equiv 1$, "antiorders" them, i.e. puts operator $\hat{a}^\dagger$ to the right of operator $\hat{a}$. "Old" coordinates q and p are then substituted back producing a Hamiltonian $h(p,q)$. Next step is to present a propagator in the following form

$$\begin{aligned} &< \ p_f, q_f \mid \exp(-i\hat{H}t/) \mid p_i, q_i > \\ &= \lim_{\nu\to\infty} 2\pi e^{\nu t/2} \int d\mu_W^\nu \exp\left[\int i\frac{1}{2}(pdq - qdp) - i\int h(p,q)dt\right], \end{aligned} \tag{6}$$

where

$$d\mu_W^\nu = N^{-1}\exp\left[-\frac{1}{2\nu}\int\left(\dot{p}^2 + \dot{q}^2\right)dt\right]\prod_t dp(t)dq(t). \tag{7}$$

can be interpreted as a Wiener measure with diffusion constant ν. We illustrate how this method works in Appendix by considering a 1d harmonic oscillator.

Now we apply the formalism described above to a special case of the system considered in [6]. The presence of a (real) magnetic field leads to a nontrivial couplings between (X,Y) and (π_x,π_y) coordinates as we show below. We consider quadratic potential and treat π_y as a coordinate and $\hat{\pi}_x$ as a momentum conjugate. The Hamiltonian is then presented as

$$\hat{H} = \frac{\hat{\pi}_x^2}{2m} + \frac{\pi_y^2}{2m} + \frac{m\gamma^2}{2}\left(X^2 + Y^2\right) + \frac{\gamma^2}{\omega_c}X\pi_y - \frac{\gamma^2}{\omega_c}Y\hat{\pi}_x + \frac{\gamma^2}{2m\omega_c^2}\left(\hat{\pi}_x^2 + \pi_y^2\right). \tag{8}$$

Combining coordinate and momentum terms we finally obtain

$$\begin{aligned} \hat{H} \ &= \ \left(\frac{m\omega_c^2}{2} + \frac{m\gamma^2}{2}\right)\left(\frac{c}{eB}\pi_y + \frac{\omega_c\gamma^2 X}{\omega_c^2 + \gamma^2}\right)^2 \\ &+ \left(\frac{1}{2m} + \frac{\gamma^2}{2m\omega_c^2}\right)\left(\hat{\pi}_x - \frac{m\omega_c\gamma^2 Y}{\omega_c^2\gamma^2}\right)^2 + \frac{m\omega_c^2\gamma^2}{2\left(\omega_c^2 + \gamma^2\right)}\left(X^2 + Y^2\right), \end{aligned} \tag{9}$$

where the last term is simply added to the energy. The solution of the Schrödinger equation with the Hamiltonian from Eq. (9) for the fast variable π_y is then easily found

$$\begin{aligned}\Psi &= N\exp\left[-\frac{M_{eff}\Omega}{2}\left(\frac{c}{eB}\pi_y+\frac{\gamma^2 X}{\omega_c^2+\gamma^2}\right)^2\right]\\ &\times H_n\left[\left(\frac{c}{eB}\pi_y+\frac{\gamma^2 X}{\omega_c^2+\gamma^2}\right)\sqrt{M_{eff}\Omega}\right]\exp\left[\frac{i\pi_y mc\omega_c\gamma^2 Y}{(\omega_c^2+\gamma^2)}\right], \quad (10)\end{aligned}$$

where the last multiplier appears due the momentum shift.

We now calculate two terms corresponding to Berry phase. It can be easily shown that $f_n(X,Y) = i < \psi_n \mid \frac{\partial}{\partial X} \mid \psi_n >= 0$ for any n due to the fact that Hermitian polynomials with different n are orthogonal with Gaussian weight. Another exercise in calculation of Hermitian functions shows that $g_n = i < \psi_n \mid \frac{\partial}{\partial Y} \mid \psi_n >= \frac{\gamma^4 X}{(\omega_c^2+\gamma^2)^2}$.

Now we write down a Lagrangian for the variables X and Y as proposed in [4].

$$L = \frac{i}{2\nu}\left(\dot{X}^2+\dot{Y}^2\right)-\frac{m\gamma^2\omega_c^2}{2}\left(X^2+Y^2\right)+\frac{m\omega_c\left(\omega_c^4+2\omega_c^2\gamma^2\right)}{2\left(\omega_c^2+\gamma^2\right)^2}\left(Y\dot{X}-X\dot{Y}\right). \quad (11)$$

where the last term was obtained after substitution of the expression for g_n and integration by parts. Eq. (11) represents a Lagrangian of a 2d electron in a harmonic oscillator well and a transverse magnetic field [13] (see also Appendix and Eq. (25)). After identifying effective frequency $\Omega'_{eff} \approx \frac{im\omega_c\nu}{2}\left(1-\frac{\gamma^4}{(\omega_c^2+\gamma^2)^2}\right)\left(1+\frac{i\gamma^2\left(\omega_c^2+\gamma^2\right)}{m\omega_c^2\nu(\omega_c^2+2\gamma^2)}\right)$ (as it is done in Appendix) and multiplying by $\exp(m\omega_c\nu t/2)$ (as was proposed in [4]) we find that the propagator

$$K \propto \frac{\exp\left[\frac{m\omega_c\nu t}{2}\right]}{\sinh\left[\Omega'_{eff}t\right]} \propto \exp\left[\frac{m\omega_c\gamma^4 t}{2\left(\omega_c^2+\gamma^2\right)^2}\nu\right], \quad (12)$$

diverges as $\nu \to \infty$ and the proposed procedure fails.

It was later realized [14] that the presence of Berry phase resulting in nonconstant magnetic field $B(1+\partial f_n/\partial Y - \partial g_n/\partial X)$ causes modification of the proper Wiener measure [15, 16]. The divergent exponential term is

now presented as

$$\exp\left[\frac{\nu}{2}\int\left(1+\frac{\partial f_n}{\partial Y}-\frac{\partial g_n}{\partial X}\right)dt\right]. \tag{13}$$

The appearance of $\exp[-\nu/2\int(\partial g_n/\partial X)dt]$ cancels exactly with the diverging term in Eq. (12).

After scrupulous consideration it became clear that to take care of diverging terms *post factum* is a wrong way. The problem was to derive the convergence factor in a 2d system with constant magnetic field *a priori*, that would not depend on the terms resembling nonuniform magnetic field which may appear in the process of calculation from integrating out some degrees of freedom. Detailed derivation of the effective propagator for the "slow" variables X and Y which takes into account the "antiordering" procedure from the very beginning has shown that in addition to the Berry phase two more terms appear in the effective action. The reason for the emergence of two additional terms is that the Brownian motion paths are continuous and *nowhere differentiable*. We describe this derivation [14] below.

After solving a Schrödinger equation for the fast variable π_y in the adiabatic approximation

$$H\left(X,Y,\hat{\pi}_x,\pi_y\right)\mid\psi_n\left(\pi_y,X,Y\right)\rangle=\epsilon_n\left(X,Y\right)\mid\psi_n\left(\pi_y,X,Y\right)\rangle \tag{14}$$

one has to substitute a resolution of unity, given by

$$\mathbf{1}=\sum_n\mid\psi_n\left(\pi_y,X,Y\right)\rangle\langle\psi_n\left(\pi_y,X,Y\right)\mid$$

with X,Y values chosen at appropriate time slices into the T-product of the propagator for X,Y:

$$\begin{aligned}&\langle X_f,Y_f,\pi_{yf},t_f\mid\exp(-i\hat{H}(t_f-t_i))\mid X_i,Y_i,\pi_{yi},t_i\rangle\\&\quad=\lim_{\nu\to\infty}2\pi e^{\nu t/2}\int dX(t)dY(t)\sum_n\psi_n^\star\left(X_f,Y_f,\pi_{yf}\right)\psi_n\left(X_i,Y_i,\pi_{yi}\right)\\&\quad\times\lim_{\delta\to0}\prod_{l=0}^N\langle\psi_n\left(X_{l+1},Y_{l+1}\right)\mid\psi_n\left(X_l,Y_l\right)\rangle e^{-i\delta\epsilon_n(X_l,Y_l)}.\end{aligned} \tag{15}$$

Usually one assumes that

$$\lim_{\delta\to 0}\prod_{l=0}^{N}\langle\psi_n\left(X_{l+1},Y_{l+1}\right)\mid\psi_n\left(X_l,Y_l\right)\rangle=\exp\left(i\int_{t_i}^{t_f}\langle\psi\left(X,Y\right)\mid\frac{d}{dt}\mid\psi\left(X,Y\right)\rangle\right). \tag{16}$$

This is indeed correct result for continuous and differentiable path $X(t), Y(t)$, but in the present regularization, the Brownian motion paths are continuous and *nowhere differentiable*. To get the right limit we observe that

$$\begin{aligned}\langle 2 \quad\mid\quad 1\rangle &= \frac{1}{2}[\langle 2\mid 1\rangle+\langle 1\mid 2\rangle]+\frac{1}{2}[\langle 2\mid 1\rangle-\langle 1\mid 2\rangle]\\ &= 1-\frac{1}{2}[\langle 2\mid(\mid 2\rangle-\mid 1\rangle)+(\langle 2\mid-\langle 1\mid)\rangle 2\mid]+\frac{1}{2}[\langle 2\mid 1\rangle-\langle 1\mid 2\rangle]\\ &= 1-\frac{1}{2}[(\langle 2\mid-\langle 1\mid)(\mid 2\rangle-\mid 1\rangle)]-\frac{1}{2}[(\langle 2\mid+\langle 1\mid)(\mid 2\rangle-\mid 1\rangle)],\end{aligned} \tag{17}$$

where we have used $\langle 1\mid 1\rangle=\langle 2\mid 2\rangle=1$. Thus, with the accuracy including square terms

$$\begin{aligned}\langle 2 \quad\mid\quad 1\rangle \simeq \exp[-\frac{1}{2}[(\langle 2\mid+\langle 1\mid)(\mid 2\rangle-\mid 1\rangle)]\\ -\frac{1}{2}[(\langle 2 \quad\mid\quad -\langle 1\mid)(\mid 2\rangle-\mid 1\rangle)]-\frac{1}{2}[\langle 2\mid(\mid 2\rangle-\mid 1\rangle)]^2]\end{aligned} \tag{18}$$

where the last term is simply a sum of the first two terms squared and multiplied by the corresponding coefficient in Taylor series. It is introduced to make both sides in Eq. (18) equal including terms of the second order. It is easy to show that the first term in the exponent indeed leads to Eq. (16) and one can use

$$\begin{aligned}i\langle\psi_n \quad\mid\quad \frac{d}{dt}\mid\psi_n\rangle &= i\langle\psi_n\mid\frac{\partial}{\partial X}\mid\psi_n\rangle\dot{X}+i\langle\psi_n\mid\frac{\partial}{\partial Y}\mid\psi_n\rangle\dot{Y}\\ &\equiv f_n(X,Y)\dot{X}+g_n(X,Y)\dot{Y}\end{aligned} \tag{19}$$

to produce expression as in [6] Two other terms in the exponent of Eq. (18) are zero for continuous and differentiable paths, but are different from zero for Brownian motion paths! For Brownian paths, where ν plays the role of diffusion constant, one has ($\delta>0$) $\langle[X(t+\delta)-X(t)]^2\rangle=\nu\delta$ (the same for Y). The second term in the exponent of Eq. (18) is then given by (one of the Ito rules)

$$-\frac{1}{2}\int dt\|d\mid\psi\rangle\|^2=-\frac{\nu}{2}\int dt\left[\|\frac{\partial\psi}{\partial X}|^2+\|\frac{\partial\psi}{\partial Y}|^2\right]. \tag{20}$$

The last term in the exponent is

$$-\frac{1}{2}\int dt \mid \langle\psi \mid d\psi\rangle \mid^2 = \frac{\nu}{2}\int dt \left(f_n^2 + g_n^2\right). \tag{21}$$

Now we have to add those three terms to the effective Lagrangian in Eq. (11). Accurate evaluation of Eq.(19)-(21) produces the following result

$$\exp\left[-\frac{\nu t m \omega_c \gamma^4}{2\left(\omega_c^2+\gamma^2\right)^2}(2n+1)\right]. \tag{22}$$

Repeating the procedure that led to Eq. (12) and multiplying the result by the correction term obtained in Eq. (22) we finally obtain for the propagator

$$\begin{aligned} K &= \lim_{\nu\to\infty}\sum_n \exp\left[-it\left(\omega_c+\frac{\gamma^2}{\omega_c}\right)\left(n+\frac{1}{2}\right)\right]\psi_n^*\left(q_f,X_f,Y_f\right)\psi_n\left(q_0,X_0,Y_0\right) \\ &\times\frac{m\omega_c\left(\omega_c^4+2\omega_c^2\gamma^2\right)}{4\pi\left(\omega_c^2+\gamma^2\right)^2}\exp\left[F(X_f,Y_f,X_0,Y_0)\right]\exp\left[-\frac{\nu t m\omega_c\gamma^4}{2\left(\omega_c^2+\gamma^2\right)^2}2n\right], \end{aligned} \tag{23}$$

where F is a regular function depending on initial and final positions. As one can see all terms with $n > 0$ vanish as ν tends to infinity. We therefore, conclude that the applied method produces correct continuum limit only for the zero Landau level.

In summary, we have considered the problem of continuum limit for path integrals in quantum systems where the operator ordering is ambiguous. We have shown that special "antiordering" procedure proved to solve the problem correctly for one-dimensional systems fails for two-dimensional systems in the perpendicular constant magnetic field. We have illustrated both results using exactly solvable models. In particular, the failure of the procedure was shown for a two dimensional electron in a harmonic potential in the presence of a perpendicular magnetic field. We can speculate that the origin of the failure for the "antiordering" procedure lies in its "by force" introduction after adiabatic expansion. On the other hand, its introduction before adiabatic expansion for all four variables, will immediately affect Schrödinger equation for the fast variables.

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Appendix

We want to illustrate a method proposed by Klauder and Daubechies in [4] by a simple example of a 1d harmonic oscillator. After introduction of the new measure and a proper "antiordering" the Lagrangian according to [4] is presented as

$$L_{1D} = \frac{i}{2\nu}(\dot{p}^2 + \dot{q}^2) + \frac{1}{2}(p\dot{q} - q\dot{p}) - \frac{1}{2}(q^2 + p^2) + \frac{1}{2}, \tag{24}$$

where additional one-half appears due to the "antiordering". If we take into account that in a coherent states representation p and q are independent then it turns out that the Lagrangian L_{1D} has the same structure as a Lagrangian for a 2d electron in a harmonic oscillator well and a transverse magnetic field mentioned above [13].

$$L_{2D} = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) + \frac{m\omega}{2}(x\dot{y} - y\dot{x}) - \frac{m\Omega^2}{2}(x^2 + y^2). \tag{25}$$

The propagator for L_{2D} is calculated exactly:

$$\begin{aligned} K(x_f, y_f, t \quad | \quad x_i, y_i, 0) = \frac{m\Omega'}{2\pi i \sin(\Omega' t)} \exp[i\frac{m\Omega'}{2\sin(\Omega' t)}(\cos(\Omega' t) \\ \times(x_f^2 + y_f^2 + x_i^2 + y_i^2) - 2\cos(\omega t/2)(x_f x_i + y_f y_i) \\ +2\sin(\omega t/2)(x_f y_i - x_i y_f))], \end{aligned} \tag{26}$$

where $\Omega' = (\Omega^2 + \frac{\omega^2}{4})^{1/2}$. Comparing Eq. (24) and Eq. (25) we find relations between the parameters of two Lagrangians: $m = i/\nu$, $\Omega^2 = -i\nu$ and $\omega = -i\nu$. For large ν we approximate $\Omega' \approx \frac{i\nu}{2} - 1$. Substituting those values into Eq. (26), multiplying expression by $\exp(\nu t/2)$ and taking the limit $\nu \to \infty$ we finally obtain

$$K(p_f, q_f, t|p_i, q_i)0) = \exp[-\frac{1}{4}(p_f^2 + q_f^2 + p_i^2 + q_i^2) + \frac{1}{2}(q_f - ip_f)(q_i + ip_i)e^{-it} - \frac{it}{2}], \tag{27}$$

which is the exact solution for a propagator of a 1d harmonic oscillator in a coherent states representation [5].

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