Variational approach to a hydrogen atom in a uniform magnetic field of arbitrary strength

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(Received 17 May 2000; published 13 October 2000)

Extending the Feynman-Kleinert variational approach, we calculate the temperature-dependent effective classical potential governing the quantum statistics of a hydrogen atom in a uniform magnetic field at all temperatures. The zero-temperature limit yields the binding energy of the electron, which is quite accurate for all magnetic-field strengths, and exhibits, in particular, correct logarithmic growth at large fields.

PACS number(s): 31.15.Pf, 03.65.Ca, 05.30.−d

I. INTRODUCTION

Quantum-statistical and -mechanical properties of a hydrogen atom in an external magnetic field are not exactly calculable. Perturbative approaches yield good results only for weak uniform fields, as discussed in detail by Le Guillou and Zinn-Justin [1], who interpolated with analytic mapping techniques the ground-state energy between weak and strong fields. Other approaches are based on recursive procedures in higher-order perturbation theory [2–4]. Zero-temperature properties were also investigated with the help of an operator optimization method in a second-quantized variational procedure [5]. The behavior at high uniform fields was inferred from treatments of the one-dimensional hydrogen atom [6–8]. Hydrogen in strong magnetic fields is still a problem under investigation, since its solution is necessary to understand the properties of white dwarfs and neutron stars, as emphasized in Refs. [9–12]. A compact and detailed presentation of the bound states and highly accurate numerically values for the energy levels is given in Ref. [13].

Equations for a first-order variational approach to the ground-state energy of hydrogen in a uniform magnetic field, based on the Jensen-Peierls inequality, were set down a long time ago [14], but never evaluated. Apparently, they merely served as a preparation for attacking the more complicated problem of a polaron in a magnetic field [14–16].

In our approach, we calculate the quantum-statistical properties of the system by an extension of variational perturbation theory [17]. The crucial quantity is the effective classical potential. In the zero-temperature limit, this yields the ground-state energy. Our calculations in a magnetic field require an extension of the formalism in Ref. [17], which derives the effective classical potential from the phase-space representation of the partition function.

Variational perturbation theory has an important advantage over other approaches: This calculation yields a good effective classical potential for *all* temperatures and coupling strengths. The quantum-statistical partition function is obtained from a simple integral over a Boltzmann factor involving the effective classical potential. The ground-state energy is then obtained from its zero-temperature limit. The asymptotic behavior in the strong-coupling limit emerges automatically, and does not have to be derived from other sources.

II. EFFECTIVE CLASSICAL REPRESENTATIONS FOR THE QUANTUM-STATISTICAL PARTITION FUNCTION

A point particle in D dimensions with a potential $V(\mathbf{x})$ and a vector potential $\mathbf{A}(\mathbf{x})$ is described by a Hamiltonian

$$H(\mathbf{p},\mathbf{x})=\frac{1}{2M}[\mathbf{p}-e\,\mathbf{A}(\mathbf{x})]^2+V(\mathbf{x}). \tag{2.1}$$

The quantum-statistical partition function is given by the Euclidean phase-space path integral

$$Z=\oint \mathcal{D}'^{D}x\mathcal{D}^{D}p\, e^{-\mathcal{A}[\mathbf{p},\mathbf{x}]/\hbar}, \tag{2.2}$$

with an action

$$\mathcal{A}[\mathbf{p},\mathbf{x}]=\int_0^{\hbar\beta} d\tau[-i\mathbf{p}(\tau)\cdot\dot{\mathbf{x}}(\tau)+H(\mathbf{p}(\tau),\mathbf{x}(\tau))], \tag{2.3}$$

and the path measure

$$\oint \mathcal{D}'^{D}x\mathcal{D}^{D}p=\lim_{N\to\infty}\prod_{n=1}^{N+1}\left[\int\frac{d^Dx_n d^Dp_n}{(2\pi\hbar)^D}\right]. \tag{2.4}$$

The parameter $\beta=1/k_BT$ denotes the usual inverse thermal energy at a temperature T, where k_B is the Boltzmann constant. From Z we obtain the free energy of the system:

$$F=-\frac{1}{\beta}\ln Z. \tag{2.5}$$

In perturbation theory, one treats the external potential $V(\mathbf{x})$ as a small quantity, and expands the partition function into powers of $V(\mathbf{x})$. Such a naive expansion is applicable only for extremely weak couplings, and has a vanishing radius of convergence. Convergence is achieved by variational perturbation theory [17], which yields good approximations for all potential strengths, as we shall see in a sequel.

A. Effective classical potential

All quantum-mechanical systems studied so far in variational perturbation theory were governed by a Hamiltonian of the standard form

$$H(\mathbf{p},\mathbf{x})=\frac{\mathbf{p}^2}{2M}+V(\mathbf{x}). \tag{2.6}$$

The simple quadratic dependence on the momenta makes the momentum integrals in the path integral (2.2) trivial. The remaining configuration space representation of the partition function is used to define an effective classical potential $V_{\rm eff}(\mathbf{x}_0)$, from which the quantum-mechanical partition function is found by a classically looking integral

$$Z=\int \frac{d^Dx_0}{\lambda_{\rm th}^D}\exp[-\beta V_{\rm eff}(\mathbf{x}_0)], \tag{2.7}$$

where $\lambda_{\rm th}=\sqrt{2\pi\hbar^2\beta/M}$ is the thermal wavelength. The Boltzmann factor plays the role of a *local partition function* $Z^{\mathbf{x}_0}$, which is calculated from the restricted path integral

$$e^{-\beta V_{\rm eff}(\mathbf{x}_0)}\equiv Z^{\mathbf{x}_0}=\lambda_{\rm th}^D\oint \mathcal{D}^Dx\,\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})e^{-\mathcal{A}[\mathbf{x}]/\hbar}, \tag{2.8}$$

with the action

$$\mathcal{A}[\mathbf{x}]=\int_0^{\hbar\beta}d\tau\left[\frac{M}{2}\dot{\mathbf{x}}^2(\tau)+V(\mathbf{x}(\tau))\right] \tag{2.9}$$

and the path measure

$$\oint \mathcal{D}^Dx=\lim_{N\to\infty}\prod_{n=1}^{N+1}\left\{\int\frac{d^Dx_n}{[2\pi\hbar^2\beta/M(N+1)]^{D/2}}\right\}. \tag{2.10}$$

The special treatment of the temporal average of the Fourier path,

$$\mathbf{x}_0=\overline{\mathbf{x}(\tau)}=\frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau\,\mathbf{x}(\tau), \tag{2.11}$$

is essential for the quality of the results. It subtracts from the harmonic fluctuation width $\langle\mathbf{x}^2\rangle^{\rm cl}$ the classical divergence proportional to $T=1/k_B\beta$ of the Dulong-Petit law [17,19]. Such diverging fluctuations cannot be treated perturbatively, and require the final integration in expression (2.7) to be done numerically. For the Coulomb potential $V(\mathbf{x})=-e^2/4\pi\varepsilon_0|\mathbf{x}|$ in three dimensions, the effective classical potential in Eq. (2.8) can be approximated well by variational perturbation theory [17,19,20].

B. Effective classical Hamiltonian

In order to deal with Hamiltonians like Eq. (2.1), which contain a $\mathbf{p}\cdot\mathbf{A}(\mathbf{x})$ term, we must generalize the variational procedure. Extending Eq. (2.8), we define an *effective classical Hamiltonian* by the phase-space path integral

$$\begin{aligned}e^{-\beta H_{\rm eff}(\mathbf{p}_0,\mathbf{x}_0)}&\equiv Z^{\mathbf{p}_0,\mathbf{x}_0}\\&=(2\pi\hbar)^D\oint\mathcal{D}'^Dx\mathcal{D}^Dp\,\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})\\&\quad\times\delta(\mathbf{p}_0-\overline{\mathbf{p}(\tau)})e^{-\mathcal{A}[\mathbf{p},\mathbf{x}]/\hbar},\end{aligned} \tag{2.12}$$

with action (2.3) and measure (2.4). This allows us to express the partition function as the classical looking phase-space integral

$$Z=\int\frac{d^Dx_0d^Dp_0}{(2\pi\hbar)^D}\exp[-\beta H_{\rm eff}(\mathbf{p}_0,\mathbf{x}_0)], \tag{2.13}$$

where $\mathbf{p}_0$ is the temporal average of the momentum:

$$\mathbf{p}_0=\overline{\mathbf{p}(\tau)}=\frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau\,\mathbf{p}(\tau). \tag{2.14}$$

The fixing of $\mathbf{p}_0$ is done for the same reason as that for $\mathbf{x}_0$, since the classical expectation value $\langle\mathbf{p}^2\rangle^{\rm cl}$ is diverging linearly with T, just as $\langle\mathbf{x}^2\rangle^{\rm cl}$.

In the special case of a standard Hamiltonian (2.6), the effective Hamiltonian in Eq. (2.13) reduces to the effective classical potential, since the momentum integral in Eq. (2.12) can then be easily performed, and the resulting restricted partition function becomes

$$Z^{\mathbf{p}_0,\mathbf{x}_0}=\exp\left(-\beta\frac{\mathbf{p}_0^2}{2M}\right)Z^{\mathbf{x}_0}, \tag{2.15}$$

with the local partition function $Z^{\mathbf{x}_0}=\exp[-\beta V_{\rm eff}(\mathbf{x}_0)]$ of Eq. (2.8). Thus the complete quantum statistical partition function is given by Eq. (2.13), with an effective classical Hamilton function

$$H_{\rm eff}(\mathbf{p}_0,\mathbf{x}_0)=\frac{\mathbf{p}_0^2}{2M}+V_{\rm eff}(\mathbf{x}_0). \tag{2.16}$$

As a consequence of the purely quadratic momentum dependence of $H(\mathbf{p},\mathbf{x})$ in Eq. (2.6), the $\mathbf{p}_0$ integral in Eq. (2.13) can be performed, thus expressing the quantum-statistical partition function as a pure configuration space integral over the Boltzmann factor involving the effective classical potential $V_{\rm eff}(\mathbf{x}_0)$, as in Eq. (2.7).

C. Exact effective classical Hamiltonian for an electron in a constant magnetic field

The effective classical Hamiltonian for the electron moving in a constant magnetic field can be calculated exactly. We consider a magnetic field $\mathbf{B}=B\mathbf{e}_z$ pointing along the positive z axis. The only nontrivial motion of the electron is in the x-y plane. In symmetric gauge the vector potential is given by

$$\mathbf{A}(\mathbf{x})=\frac{B}{2}(-y,x,0). \tag{2.17}$$

The choice of the gauge does not affect the partition function since the periodic path integral [Eq. (2.2)] is gauge invariant. Ignoring the trivial free particle motion along the z direction, we may restrict our attention to the two-dimensional Hamiltonian

$$H(\mathbf{p},\mathbf{x})=\frac{\mathbf{p}^2}{2M}-\omega_B l_z(\mathbf{p},\mathbf{x})+\frac{1}{2}M\omega_B^2\mathbf{x}^2, \tag{2.18}$$

with $\mathbf{x}=(x,y)$ and $\mathbf{p}=(p_x,p_y)$. Here $\omega_B=eB/2M$ is half the Landau frequency, and

$$l_z(\mathbf{p},\mathbf{x})=(\mathbf{x}\times\mathbf{p})_z=xp_y-yp_x \tag{2.19}$$

is the third component of the orbital angular momentum.

It is useful at intermediate stages of the following development to treat the more general problem

$$H(\mathbf{p},\mathbf{x})=\frac{\mathbf{p}^2}{2M}-\omega_B l_z(\mathbf{p},\mathbf{x})+\frac{1}{2}M\Omega_\perp^2\mathbf{x}^2. \tag{2.20}$$

At the end of the calculation, only the limit $\Omega_\perp\to\omega_B$ will be relevant. The partition function of the problem is given by Eq. (2.13), with $D=2$. Being interested in an effective classical formulation, we have to calculate the path integral (2.12). First we express the δ function for the averaged momentum as a Fourier integral

$$\delta(\mathbf{p}_0-\overline{\mathbf{p}(\tau)})=\int\frac{d^2\xi}{(2\pi\hbar)^2}\exp\left(-\frac{i}{\hbar}\boldsymbol{\xi}\cdot\mathbf{p}_0\right)\times\exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\,\mathbf{v}_0(\boldsymbol{\xi})\cdot\mathbf{p}(\tau)\right] \tag{2.21}$$

involving an auxiliary source

$$\mathbf{v}_0(\boldsymbol{\xi})=-\frac{i}{\hbar\beta}\boldsymbol{\xi}, \tag{2.22}$$

which is constant in time. Substituting the δ function in Eq. (2.12) by this source representation, the partition function reads

$$Z^{\mathbf{p}_0,\mathbf{x}_0}=\int d^2\xi\exp\left(-\frac{i}{\hbar}\boldsymbol{\xi}\cdot\mathbf{p}_0\right)\oint\mathcal{D}'^2x\mathcal{D}^2p\,\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})\times\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau[-i\mathbf{p}(\tau)\cdot\dot{\mathbf{x}}(\tau)+H(\mathbf{p}(\tau),\mathbf{x}(\tau))+\mathbf{v}_0(\boldsymbol{\xi})\cdot\mathbf{p}(\tau)]\right\}. \tag{2.23}$$

Evaluating the momentum integrals and utilizing the periodicity property $\mathbf{x}(0)=\mathbf{x}(\hbar\beta)$, we obtain the configuration space path integral

$$Z^{\mathbf{p}_0,\mathbf{x}_0}=\int d^2\xi\exp\left(-\frac{i}{\hbar}\boldsymbol{\xi}\cdot\mathbf{p}_0-\frac{M}{2\hbar^2\beta}\boldsymbol{\xi}^2\right)\times\oint\mathcal{D}^2x\,\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})\times\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\left[\frac{M}{2}\dot{\mathbf{x}}^2(\tau)+\frac{1}{2}M(\Omega_\perp^2-\omega_B^2)\mathbf{x}^2(\tau)-iM\omega_B[\mathbf{x}(\tau)\times\dot{\mathbf{x}}(\tau)]_z+\mathbf{x}(\tau)\cdot\mathbf{j}_1(\boldsymbol{\xi})\right]\right\}, \tag{2.24}$$

where the source $\mathbf{v}_0$ coupled to the momentum in Eq. (2.23) has turned to a source $\mathbf{j}_1$ coupled to the path in configuration space [21], with components

$$\mathbf{j}_1(\boldsymbol{\xi})=M\omega_B(v_{0y}(\boldsymbol{\xi}),-v_{0x}(\boldsymbol{\xi}))=\frac{i\omega_B M}{\hbar\beta}(-\xi_y,\xi_x). \tag{2.25}$$

Expressing the δ function in the path integral of Eq. (2.24) by the Fourier integral

$$\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})=\int\frac{d^2\kappa}{(2\pi)^2}\exp\left(i\boldsymbol{\kappa}\cdot\mathbf{x}_0\right)\times\exp\left[-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\,\mathbf{j}_2(\boldsymbol{\kappa})\cdot\mathbf{x}(\tau)\right] \tag{2.26}$$

with the new source

$$\mathbf{j}_2(\boldsymbol{\kappa})=\frac{i\boldsymbol{\kappa}}{\beta}, \tag{2.27}$$

the partition function (2.24) can be written as

$$Z^{\mathbf{p}_0,\mathbf{x}_0}=\int d^2\xi\exp\left(-\frac{i}{\hbar}\boldsymbol{\xi}\cdot\mathbf{p}_0-\frac{M}{2\hbar^2\beta}\boldsymbol{\xi}^2\right)\times\int\frac{d^2\kappa}{(2\pi)^2}\exp\left(i\boldsymbol{\kappa}\cdot\mathbf{x}_0\right)Z_\Omega[\mathbf{J}(\boldsymbol{\xi},\boldsymbol{\kappa})]. \tag{2.28}$$

The functional $Z_\Omega[\mathbf{J}(\boldsymbol{\xi},\boldsymbol{\kappa})]$ is defined as the configuration space path integral

$$Z_\Omega[\mathbf{J}(\boldsymbol{\xi},\boldsymbol{\kappa})]=\oint\mathcal{D}^2x\exp\left[-\frac{1}{2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\times\mathbf{x}(\tau)\mathbf{G}^{-1}(\tau,\tau')\mathbf{x}(\tau')-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\,\mathbf{J}(\boldsymbol{\xi},\boldsymbol{\kappa})\cdot\mathbf{x}(\tau)\right], \tag{2.29}$$

where we have introduced the combined source $\mathbf{J}(\boldsymbol{\xi},\boldsymbol{\kappa})=\mathbf{j}_1(\boldsymbol{\xi})+\mathbf{j}_2(\boldsymbol{\kappa})$. Formally, the solution reads

$$Z_\Omega[\mathbf{J}(\boldsymbol{\xi},\boldsymbol{\kappa})]=Z_\Omega[0]\exp\left[\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,\mathbf{J}(\boldsymbol{\xi},\boldsymbol{\kappa})\times\mathbf{G}(\tau,\tau')\mathbf{J}(\boldsymbol{\xi},\boldsymbol{\kappa})\right], \tag{2.30}$$

where $\mathbf{G}(\tau,\tau')$ is the matrix of Green functions obtained by inverting the kernel

$$\mathbf{G}^{-1}(\tau,\tau')=\frac{M}{\hbar}\begin{pmatrix}-\frac{d^2}{d\tau^2}+\Omega_\perp^2-\omega_B^2 & -2i\omega_B\frac{d}{d\tau}\\ 2i\omega_B\frac{d}{d\tau} & -\frac{d^2}{d\tau^2}+\Omega_\perp^2-\omega_B^2\end{pmatrix}\times\delta(\tau-\tau'). \tag{2.31}$$

The inversion is easily done in frequency space after spectrally decomposing the δ function into the Matsubara frequencies $\omega_m=2\pi m/\hbar\beta$:

$$\delta(\tau-\tau')=\frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}e^{i\omega_m(\tau-\tau')}. \tag{2.32}$$

The result is

$$\tilde{\mathbf{G}}(\omega_m)=\frac{\hbar}{M}\frac{1}{\det\tilde{\mathbf{G}}}\begin{pmatrix}\omega_m^2+\Omega_\perp^2-\omega_B^2 & -2\omega_B\omega_m\\ 2\omega_B\omega_m & \omega_m^2+\Omega_\perp^2-\omega_B^2\end{pmatrix}. \tag{2.33}$$

At this point, the additional oscillator in Eq. (2.24) proves useful: It ensures that the determinant

$$\det\tilde{\mathbf{G}}(\omega_m)=(\omega_m^2+\Omega_\perp^2-\omega_B^2)^2+4\omega_B^2\omega_m^2 \tag{2.34}$$

is nonzero for $m=0$, thus playing the role of an infrared regulator. The Fourier expansion

$$\mathbf{G}(\tau,\tau')=\frac{1}{\hbar\beta}\sum_{m=-\infty}^{\infty}\tilde{\mathbf{G}}(\omega_m)e^{-i\omega_m(\tau-\tau')} \tag{2.35}$$

yields the matrix of the Green functions,

$$\mathbf{G}(\tau,\tau')=\begin{pmatrix}G_{xx}(\tau,\tau') & G_{xy}(\tau,\tau')\\ G_{yx}(\tau,\tau') & G_{yy}(\tau,\tau')\end{pmatrix} \tag{2.36}$$

which inherits the symmetry properties from the kernel (2.31):

$$G_{xx}(\tau,\tau')=G_{yy}(\tau,\tau'),\quad G_{xy}(\tau,\tau')=-G_{yx}(\tau,\tau'). \tag{2.37}$$

A more detailed description of these Green functions is given in Appendixes A and B.

Since the current $\mathbf{J}$ does not depend on the Euclidean time, expression (2.30) therefore simplifies to

$$Z_\Omega[\mathbf{J}(\boldsymbol{\xi},\boldsymbol{\kappa})]=Z_\Omega[0]\exp\left[-\frac{1}{\hbar^2}\mathbf{J}^2(\boldsymbol{\xi},\boldsymbol{\kappa})\times\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,G_{xx}(\tau,\tau')\right]. \tag{2.38}$$

The Green function has the Fourier decomposition

$$G_{xx}(\tau,\tau')=\frac{1}{M\beta}\sum_{m=-\infty}^{\infty}\frac{\omega_m^2+\Omega_\perp^2-\omega_B^2}{(\omega_m^2+\Omega_+^2)(\omega_m^2+\Omega_-^2)}e^{-i\omega_m(\tau-\tau')}, \tag{2.39}$$

where $\Omega_\pm$ are the frequencies,

$$\Omega_\pm=\Omega_\perp\pm\omega_B, \tag{2.40}$$

and $\Omega_\perp>\omega_B$, for stability.

The ratios in the sum of Eq. (2.39) can be decomposed into two partial fractions, each of them representing a single harmonic oscillator with frequencies Ω_+ and Ω_-, respectively. The analytic form of the periodic Green function of a single harmonic oscillator is well known (see Chapter 3 in Ref. [17]), and for the present Green function (2.39) we obtain

$$G_{xx}(\tau,\tau')=\frac{\hbar}{4M\Omega_\perp}\left(\frac{\cosh\Omega_+(|\tau-\tau'|-\hbar\beta/2)}{\sinh\hbar\beta\Omega_+/2}+\frac{\cosh\Omega_-(|\tau-\tau'|-\hbar\beta/2)}{\sinh\hbar\beta\Omega_-/2}\right). \tag{2.41}$$

By writing the determinant (2.34) as

$$\det\tilde{\mathbf{G}}(\omega_m)=(\omega_m^2+\Omega_+^2)(\omega_m^2+\Omega_-^2) \tag{2.42}$$

and summing over the logarithms of this, we calculate the partition function as a product of two single harmonic oscillators:

$$Z_\Omega=Z_\Omega[0]=\frac{1}{2\sinh\hbar\beta\Omega_+/2}\frac{1}{2\sinh\hbar\beta\Omega_-/2}. \tag{2.43}$$

Results (2.41) and (2.43) determine the generating functional (2.38). The Euclidean time integrations are then easily done, and subsequently the $\boldsymbol{\kappa}$ and $\boldsymbol{\xi}$ integrations in Eq. (2.28). As a result, we obtain the restricted partition function

$$Z^{\mathbf{p}_0,\mathbf{x}_0}=\exp\left\{-\beta\left(-\frac{1}{\beta}\ln\frac{\sinh\hbar\beta\Omega_+/2}{\hbar\beta\Omega_+/2}\frac{\sinh\hbar\beta\Omega_-/2}{\hbar\beta\Omega_-/2}+\frac{\mathbf{p}_0^2}{2M}-\omega_B l_z(\mathbf{p}_0,\mathbf{x}_0)+\frac{1}{2}M\Omega_\perp^2\mathbf{x}_0^2\right)\right\}. \tag{2.44}$$

Taking the limit $\Omega_\perp\to\omega_B$, from Eq. (2.40) we find $\Omega_+\to 2\omega_B$ and $\Omega_-\to 0$, and therefore

$$\lim_{\Omega_\perp \to \omega_B} \frac{\sinh \hbar\beta\Omega_+/2}{\hbar\beta\Omega_+/2} = \frac{\sinh \hbar\beta\omega_B}{\hbar\beta\omega_B},$$

$$\lim_{\Omega_\perp \to \omega_B} \frac{\sinh \hbar\beta\Omega_-/2}{\hbar\beta\Omega_-/2} = 1. \tag{2.45}$$

Recalling definition (2.12), we identify the exact effective classical Hamiltonian for an electron in a magnetic field as

$$H_{\rm eff}(\mathbf{p}_0,\mathbf{x}_0) = \frac{1}{\beta}\ln\frac{\sinh \hbar\beta\omega_B}{\hbar\beta\omega_B} + \frac{\mathbf{p}_0^2}{2M} - \omega_B l_z(\mathbf{p}_0,\mathbf{x}_0) + \frac{1}{2}M\omega_B^2\mathbf{x}_0^2. \tag{2.46}$$

Integrating out the momenta in Eq. (2.13), the configuration space representation (2.7) for the partition function contains the effective classical potential for a charged particle in the plane perpendicular to the direction of a uniform magnetic field:

$$V_{\rm eff}(\mathbf{x}_0) = \frac{1}{\beta}\ln\frac{\sinh \hbar\beta\omega_B}{\hbar\beta\omega_B}. \tag{2.47}$$

Note that this is a constant potential.

Denoting the area $\int d^2x_0$ by A, we find the exact quantum-statistical partition function

$$Z = \frac{A}{\lambda_{\rm th}^2}\frac{\hbar\beta\omega_B}{\sinh \hbar\beta\omega_B}. \tag{2.48}$$

After these preparations, we can turn our attention to the system we want to study in this paper: the hydrogen atom in a uniform magnetic field, where the additional Coulomb interaction prevents us from finding an exact solution for the effective classical Hamilton function.

III. HYDROGEN ATOM IN CONSTANT MAGNETIC FIELD

The zero-temperature properties of the hydrogen atom without external fields are exactly known. For the quantum statistics at finite temperatures, an analytical expression exists, but it is hard to evaluate. It is easier to find an accurate approximate result with the help of variational perturbation theory [20]. Similar calculations have been performed for the electron-proton pair distribution function which can be interpreted as the unnormalized density matrix [19].

Here we extend this method of calculation to the hydrogen atom in a constant magnetic field. This extension is quite nontrivial, since the weak- and strong-field limits will turn out to exhibit completely different asymptotic behaviors. Let us first generalize variational perturbation theory to an electron in a constant magnetic field and arbitrary potential.

A. Generalized variational perturbation theory

We consider once more the effective classical form (2.13) of the quantum-statistical partition function, which requires a path integration (2.12) in phase space. Fluctuations parallel and vertical to the magnetic-field lines are now both nontrivial; we must deal with a full three-dimensional system, and the components of the electron position and momentum are now denoted by $\mathbf{x}=(x,y,z)$ and $\mathbf{p}=(p_x,p_y,p_z)$. For a uniform magnetic field pointing along the z axis, the vector potential $\mathbf{A}(\mathbf{x})$ is used in the gauge (2.17). Thus the Hamilton function of an electron in a magnetic field and an arbitrary potential $V(\mathbf{x})$ is

$$H(\mathbf{p},\mathbf{x}) = \frac{\mathbf{p}^2}{2M} - \omega_B l_z(\mathbf{p},\mathbf{x}) + \frac{1}{2}M\omega_B^2\mathbf{x}^2 + V(\mathbf{x}). \tag{3.1}$$

The orbital angular momentum $l_z(\mathbf{p},\mathbf{x})$ was introduced in Eq. (2.19), and the frequency ω_B below Eq. (2.18). The importance of the separation of the zero-frequency components $\mathbf{x}_0$ and $\mathbf{p}_0$ was discussed in Sec. II. Their divergence with the temperature T prevents a perturbative treatment. Thus it is essential to set up a perturbation theory only for the fluctuations around $\mathbf{x}_0$ and $\mathbf{p}_0$. For this we rewrite the action functional (2.3) associated with Hamiltonian (3.1) as

$$\mathcal{A}[\mathbf{p},\mathbf{x}] = \mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x}] + \mathcal{A}_{\rm int}[\mathbf{p},\mathbf{x}], \tag{3.2}$$

where we have introduced the fluctuation action

$$\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x}] = \int_0^{\hbar\beta} d\tau \Big\{ -i[\mathbf{p}(\tau)-\mathbf{p}_0]\cdot\dot{\mathbf{x}}(\tau) + \frac{1}{2M}[\mathbf{p}(\tau)-\mathbf{p}_0]^2 - \Omega_B l_z(\mathbf{p}(\tau) - \mathbf{p}_0, \mathbf{x}(\tau)-\mathbf{x}_0) + \frac{1}{2}M\Omega_\perp^2[\mathbf{x}^\perp(\tau)-\mathbf{x}_0^\perp]^2 + \frac{1}{2}M\Omega_\parallel^2[z(\tau)-z_0]^2 \Big\}, \tag{3.3}$$

in which $\mathbf{x}^\perp=(x,y)$ denotes the transverse part of $\mathbf{x}$ and $\Omega_\perp > \Omega_B$, for stability. The interaction is now

$$\mathcal{A}_{\rm int}[\mathbf{p},\mathbf{x}] = \int_0^{\hbar\beta} d\tau V_{\rm int}(\mathbf{p}(\tau),\mathbf{x}(\tau)) = \mathcal{A}[\mathbf{p},\mathbf{x}] - \mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x}], \tag{3.4}$$

with the interaction potential

$$V_{\rm int}(\mathbf{p}(\tau),\mathbf{x}(\tau)) = \frac{1}{2M}\{\mathbf{p}^2(\tau) - [\mathbf{p}(\tau)-\mathbf{p}_0]^2\} - \omega_B\mathbf{x}^\perp(\tau) \times \mathbf{p}^\perp(\tau) + \Omega_B(\mathbf{x}^\perp(\tau)-\mathbf{x}_0^\perp)\times(\mathbf{p}^\perp(\tau)-\mathbf{p}_0^\perp) + \frac{1}{2}M\omega_B^2\mathbf{x}^{\perp 2}(\tau) - \frac{1}{2}M\Omega_\perp^2[\mathbf{x}^\perp(\tau)-\mathbf{x}_0^\perp]^2 - \frac{1}{2}M\Omega_\parallel^2[z(\tau)-z_0]^2 + V(\mathbf{x}(\tau)), \tag{3.5}$$

where $\mathbf{p}^\perp=(p_x,p_y)$. The frequencies $\mathbf{\Omega}=(\Omega_B,\Omega_\perp,\Omega_\parallel)$ are arbitrary for the moment. The decomposition (3.2)

forms the basis for the variational approach, where the first term in action (3.2) allows an exact treatment. The transverse part was given in Sec. II C, and the longitudinal part is trivial, since it is harmonic with frequency $\Omega_\parallel$. The associated partition function is given by the path integral

$$Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0} = \oint \mathcal{D}'^3x\mathcal{D}^3p\,\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)}) \times \delta(\mathbf{p}_0-\overline{\mathbf{p}(\tau)})e^{-\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x}]/\hbar}, \tag{3.6}$$

which can be performed. Details are given in Appendix C. The result is

$$Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0} = \frac{\hbar\beta\Omega_+/2}{\sinh\hbar\beta\Omega_+/2}\frac{\hbar\beta\Omega_-/2}{\sinh\hbar\beta\Omega_-/2}\frac{\hbar\beta\Omega_\parallel/2}{\sinh\hbar\beta\Omega_\parallel/2}, \tag{3.7}$$

where auxiliary frequencies are composed of the frequencies Ω_B and $\Omega_\perp$ in action (3.3) as

$$\Omega_\pm(\Omega_B,\Omega_\perp) = \Omega_\perp \pm \Omega_B. \tag{3.8}$$

This partition function serves in the subsequent pertubation expansion as a trial system which depends explicitly on the frequencies $\mathbf{\Omega}$. The correlation functions are a straightforward generalization of Eq. (2.36) to three dimensions:

$$\mathbf{G}^{\mathbf{x}_0}(\tau,\tau') = \begin{pmatrix} G_{xx}^{\mathbf{x}_0}(\tau,\tau') & G_{xy}^{\mathbf{x}_0}(\tau,\tau') & 0 \\ G_{yx}^{\mathbf{x}_0}(\tau,\tau') & G_{yy}^{\mathbf{x}_0}(\tau,\tau') & 0 \\ 0 & 0 & G_{zz}^{\mathbf{x}_0}(\tau,\tau') \end{pmatrix}, \tag{3.9}$$

whose explicit form is derived in Appendix C.

The $\mathbf{\Omega}$-dependent action in Eq. (3.2) is treated perturbatively. Writing the partition function (2.12) as

$$Z^{\mathbf{p}_0,\mathbf{x}_0} = (2\pi\hbar)^3 \oint \mathcal{D}'^3x\mathcal{D}^3p\,\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})\delta(\mathbf{p}_0-\overline{\mathbf{p}(\tau)}) \times\exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x}]\right\} \times\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau V_{\rm int}(\mathbf{p}(\tau),\mathbf{x}(\tau))\right\}, \tag{3.10}$$

the second exponential is expanded into a Taylor series, yielding

$$Z^{\mathbf{p}_0,\mathbf{x}_0} = (2\pi\hbar)^3 \oint \mathcal{D}'^3x\mathcal{D}^3p\,\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})\delta(\mathbf{p}_0-\overline{\mathbf{p}(\tau)}) \times\exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x}]\right\} \times\left[1-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau V_{\rm int}(\mathbf{p}(\tau),\mathbf{x}(\tau)) + \frac{1}{2!\hbar^2}\int_0^{\hbar\beta}d\tau_1\int_0^{\hbar\beta}d\tau_2 V_{\rm int}(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1)) \times V_{\rm int}(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))-\cdots\right]. \tag{3.11}$$

Defining harmonic expectation values with respect to the restricted path integral as

$$\langle\cdots\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0} = \frac{(2\pi\hbar)^3}{Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}}\oint \mathcal{D}'^3x\mathcal{D}^3p\ \ldots\ \delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)}) \times\delta(\mathbf{p}_0-\overline{\mathbf{p}(\tau)})\exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x}]\right\}, \tag{3.12}$$

the perturbation expansion for the partition function (3.11) reads

$$Z^{\mathbf{p}_0,\mathbf{x}_0} = Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\sum_{n=0}^{\infty}\frac{(-1)^n}{\hbar^n n!} \times\left\langle\left(\int_0^{\hbar\beta}d\tau\, V_{\rm int}(\mathbf{p}(\tau),\mathbf{x}(\tau))\right)^n\right\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}. \tag{3.13}$$

This power series expansion can be rewritten in the exponential form

$$Z^{\mathbf{p}_0,\mathbf{x}_0} = Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\exp\left\{\sum_{n=0}^{\infty}\frac{(-1)^n}{\hbar^n n!} \times\left\langle\left(\int_0^{\hbar\beta}d\tau\, V_{\rm int}(\mathbf{p}(\tau),\mathbf{x}(\tau))\right)^n\right\rangle_{\mathbf{\Omega},c}^{\mathbf{p}_0,\mathbf{x}_0}\right\}, \tag{3.14}$$

where the subscript c on the expectation values indicates cumulants. The lowest cumulants are related to the full expectation values as follows:

$$\begin{aligned} &\langle O_1(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\rangle_{\mathbf{\Omega},c}^{\mathbf{p}_0,\mathbf{x}_0} = \langle O_1(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0},\\ &\langle O_1(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))O_2(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))\rangle_{\mathbf{\Omega},c}^{\mathbf{p}_0,\mathbf{x}_0}\\ &\quad = \langle O_1(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))O_2(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\\ &\qquad -\langle O_1(\mathbf{p}(\tau_1),\mathbf{x}(\tau_1))\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\langle O_2(\mathbf{p}(\tau_2),\mathbf{x}(\tau_2))\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0},\\ &\quad \vdots, \end{aligned} \tag{3.15}$$

where $O_i(\mathbf{p}(\tau_j),\mathbf{x}(\tau_j))$ denotes any observable depending on momentum and position. Recalling relation (2.12) between partition function (3.14) and effective classical Hamiltonian $H_{\rm eff}(\mathbf{p}_0,\mathbf{x}_0)$, from Eq. (3.14) we obtain the effective classical Hamiltonian as a cumulant expansion:

$$H_{\rm eff}(\mathbf{p}_0,\mathbf{x}_0)=-\frac{1}{\beta}\ln Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}+\frac{1}{\beta}\sum_{n=1}^{\infty}\frac{(-1)^n}{\hbar^n n!}\times\left\langle\left(\int_0^{\hbar\beta}d\tau\,V_{\rm int}(\mathbf{p}(\tau),\mathbf{x}(\tau))\right)^n\right\rangle_{\mathbf{\Omega},c}^{\mathbf{p}_0,\mathbf{x}_0}. \tag{3.16}$$

Up to now, we did not make any approximation. The expansion on the right-hand side is an exact expression for the effective classical Hamiltonian for any $\mathbf{\Omega}$.

For systems with a nontrivial interaction, we are capable of calculating only some initial truncated part of series (3.16), say up to the Nth order, leading to the approximate effective classical Hamiltonian

$$\mathcal{H}_{\mathbf{\Omega}}^{(N)}(\mathbf{p}_0,\mathbf{x}_0)=-\frac{1}{\beta}\ln Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}+\frac{1}{\beta}\sum_{n=1}^{N}\frac{(-1)^n}{\hbar^n n!}\times\left\langle\left(\int_0^{\hbar\beta}d\tau\,V_{\rm int}(\mathbf{p}(\tau),\mathbf{x}(\tau))\right)^n\right\rangle_{\mathbf{\Omega},c}^{\mathbf{p}_0,\mathbf{x}_0}. \tag{3.17}$$

This depends explicitly on the three parameters $\mathbf{\Omega}$. Since the exact expression (3.16) is independent of $\mathbf{\Omega}$, the best approximation for $\mathcal{H}_{\mathbf{\Omega}}^{(N)}(\mathbf{p}_0,\mathbf{x}_0)$ should depend on $\mathbf{\Omega}$ *minimally*. Thus the optimal solution will be found by determining the parameters from the conditions

$$\nabla_{\mathbf{\Omega}}\mathcal{H}_{\mathbf{\Omega}}^{(N)}(\mathbf{p}_0,\mathbf{x}_0)\overset{!}{=}0. \tag{3.18}$$

Let us denote the optimal variational parameters to Nth order by

$$\mathbf{\Omega}^{(N)}=(\Omega_B^{(N)}(\mathbf{p}_0,\mathbf{x}_0),\Omega_\perp^{(N)}(\mathbf{p}_0,\mathbf{x}_0),\Omega_\parallel^{(N)}(\mathbf{p}_0,\mathbf{x}_0)). \tag{3.19}$$

Inserting these into Eq. (3.17) yields the optimal effective classical Hamiltonian $\mathcal{H}^{(N)}(\mathbf{p}_0,\mathbf{x}_0)$.

B. First-order effective classical potential

The first-order approximation of the effective classical Hamiltonian (3.17) reads

$$\mathcal{H}_{\mathbf{\Omega}}^{(1)}(\mathbf{p}_0,\mathbf{x}_0)=-\frac{1}{\beta}\ln Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}-\langle V_{\rm int}(\mathbf{p},\mathbf{x})\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}. \tag{3.20}$$

The invariance of the system under time translations makes one of the time integrals in expansion (3.16) trivial, yielding merely an overall factor $\hbar\beta$. In particular, the first-order expectation value of $V_{\rm int}(\mathbf{x})$ in Eq. (3.20) is independent of the Euclidean time τ.

In order to calculate $\mathcal{H}_{\mathbf{\Omega}}^{(1)}(\mathbf{p}_0,\mathbf{x}_0)$, we use the two-point correlation functions derived in Appendix C, and the vanishing of the linear expectations, e.g.,

$$\langle p_x(\tau)-p_{0x}\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=0, \tag{3.21}$$

to find

$$\mathcal{H}_{\mathbf{\Omega}}^{(1)}(\mathbf{p}_0,\mathbf{x}_0)=\frac{\mathbf{p}_0^2}{2M}-\omega_B l_z(\mathbf{p}_0,\mathbf{x}_0)+\frac{1}{2}M\omega_B^2(x_0^2+y_0^2)+W_{\mathbf{\Omega}}^{(1)}(\mathbf{x}_0), \tag{3.22}$$

where we have collected all terms depending on the variational parameters $\mathbf{\Omega}$ in the potential

$$W_{\mathbf{\Omega}}^{(1)}(\mathbf{x}_0)=-\frac{1}{\beta}\ln Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}-M\Omega_B(\omega_B-\Omega_B)\,b_\perp^2(\mathbf{x}_0)+M(\omega_B^2-\Omega_\perp^2)\,a_\perp^2(\mathbf{x}_0)-\frac{1}{2}M\Omega_\parallel^2 a_\parallel^2(\mathbf{x}_0)+\langle V(\mathbf{x})\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}. \tag{3.23}$$

The quantities $a_\perp^2(\mathbf{x}_0),a_\parallel^2(\mathbf{x}_0)$, and $b_\perp^2(\mathbf{x}_0)$ are the transverse and longitudinal fluctuation widths

$$a_\perp^2(\mathbf{x}_0)=G_{xx}^{\mathbf{p}_0,\mathbf{x}_0}(0),\quad a_\parallel^2(\mathbf{x}_0)=G_{zz}^{\mathbf{p}_0,\mathbf{x}_0}(0),\quad b_\perp^2(\mathbf{x}_0)=\frac{2}{M\Omega_B}G_{xp_y}^{\mathbf{p}_0,\mathbf{x}_0}(0). \tag{3.24}$$

Note that potential (3.23) is independent of $\mathbf{p}_0$. This means that approximation (3.22) of the effective classical Hamiltonian contains no coupling of the momentum $\mathbf{p}_0$ to a variational parameter $\mathbf{\Omega}$, such that the optimal $\mathbf{\Omega}^{(1)}$ determined by minimizing $\mathcal{H}_{\mathbf{\Omega}}^{(1)}(\mathbf{p}_0,\mathbf{x}_0)$ is independent of $\mathbf{p}_0$. We may therefore integrate out $\mathbf{p}_0$ in the phase-space representation of the first-order approximation for the partition function

$$Z^{(1)}=\int\frac{d^3x_0d^3p_0}{(2\pi\hbar^3)}e^{-\beta\mathcal{H}_{\mathbf{\Omega}}^{(1)}(\mathbf{p}_0,\mathbf{x}_0)} \tag{3.25}$$

to find the pure configuration space integral

$$Z^{(1)}=\int\frac{d^3x_0}{\lambda_{\rm th}^3}e^{-\beta W_{\mathbf{\Omega}}^{(1)}(\mathbf{x}_0)}, \tag{3.26}$$

in which $W_{\mathbf{\Omega}}^{(1)}(\mathbf{x}_0)$ is the first-order approximation to the effective classical potential of an electron in a potential $V(\mathbf{x})$ and a uniform magnetic field.

C. Application to the hydrogen atom in a magnetic field

We now apply the formulas of Sec. III B to Hamiltonian (3.1) with an attracting Coulomb potential

$$V(\mathbf{x})=-\frac{e^2}{4\pi\varepsilon_0|\mathbf{x}|}, \tag{3.27}$$

where $|\mathbf{x}|$ is the distance between the electron and the proton. The only nontrivial problem is the calculation of the expectation value $\langle V(\mathbf{x}(\tau))\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}$ in Eq. (3.23). This is done using the so-called *smearing formula*, which is a Gaussian convolution of $V(\mathbf{x})$. This formula was first derived by Feynman and Kleinert [18], and now also exists in an extension to

arbitrary order [19,20]. The generalization to position- and-momentum dependent observables was given in the phase-space formulation [21]. We briefly rederive the first-order smearing formula. The expectation value is defined by

$$\langle V(\mathbf{x}(\tau'))\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=\frac{(2\pi\hbar)^3}{Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}}\oint \mathcal{D}'^3x\mathcal{D}^3p\; V(\mathbf{x}(\tau'))\;\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})\,\delta(\mathbf{p}_0-\overline{\mathbf{p}(\tau)})e^{-\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x}]/\hbar}. \tag{3.28}$$

Now we substitute the potential with the expression

$$\begin{aligned}V(\mathbf{x}(\tau'))&=\int d^3x\; V(\mathbf{x})\,\delta(\mathbf{x}-\mathbf{x}(\tau'))\\&=\int d^3x\; V(\mathbf{x})\int\frac{d^3\kappa}{(2\pi)^3}\exp[\,i\boldsymbol{\kappa}\cdot(\mathbf{x}-\mathbf{x}_0)\,]\\&\quad\times\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\,\mathbf{j}(\tau)\cdot[\mathbf{x}(\tau)-\mathbf{x}_0]\right\},\end{aligned} \tag{3.29}$$

where we have introduced the source

$$\mathbf{j}(\tau)=i\hbar\boldsymbol{\kappa}\delta(\tau-\tau'). \tag{3.30}$$

Inserting expression (3.29) into Eq. (3.28), we obtain

$$\langle V(\mathbf{x}(\tau'))\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=\frac{1}{Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}}\int d^3x\; V(\mathbf{x})\int\frac{d^3\kappa}{(2\pi)^3}\times\exp[\,i\boldsymbol{\kappa}\cdot(\mathbf{x}-\mathbf{x}_0)\,]\;Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j}], \tag{3.31}$$

with the harmonic generating functional

$$\begin{aligned}Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j}]&=(2\pi\hbar)^3\oint\mathcal{D}'^3x\mathcal{D}^3p\;\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})\\&\quad\times\delta(\mathbf{p}_0-\overline{\mathbf{p}(\tau)})\exp\left\{-\frac{1}{\hbar}\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x}]\right.\\&\quad\left.-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\,\mathbf{j}(\tau)\cdot[\mathbf{x}(\tau)-\mathbf{x}_0]\right\}.\end{aligned} \tag{3.32}$$

The solution is

$$Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j}]=Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\exp\left[\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\;\mathbf{j}(\tau)\times\mathbf{G}^{\mathbf{x}_0}(\tau,\tau')\;\mathbf{j}(\tau')\right], \tag{3.33}$$

with the 3×3 matrix of the Green functions of Eq. (3.9). The properties of the Green functions are discussed in Appendixes A and B. Expressing the source $\mathbf{j}(\tau)$ in terms of $\boldsymbol{\kappa}$ via Eq. (3.30), and performing the τ integrations, we arrive at

$$\langle V(\mathbf{x}(\tau'))\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=\int d^3x\; V(\mathbf{x})\int\frac{d^3\kappa}{(2\pi)^3}\exp\{i\boldsymbol{\kappa}\cdot[\mathbf{x}-\mathbf{x}_0]\}\times\exp\left[-\frac{1}{2}\boldsymbol{\kappa}\mathbf{G}^{\mathbf{x}_0}(0)\;\boldsymbol{\kappa}\right]. \tag{3.34}$$

Recognizing that $G_{yx}^{\mathbf{x}_0}(0)=G_{xy}^{\mathbf{x}_0}(0)$ vanish, the $\boldsymbol{\kappa}$ integral is easily calculated, and leads to the first-order smearing formula for an arbitrary position-dependent potential

$$\begin{aligned}\langle V(\mathbf{x}(\tau'))\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}&=\frac{1}{(2\pi)^{3/2}a_\perp^2(\mathbf{x}_0)\sqrt{a_\parallel^2(\mathbf{x}_0)}}\int d^3x\; V(\mathbf{x})\\&\quad\times\exp\left[-\frac{(x-x_0)^2+(y-y_0)^2}{2a_\perp^2(\mathbf{x}_0)}\right.\\&\quad\left.-\frac{(z-z_0)^2}{2a_\parallel^2(\mathbf{x}_0)}\right],\end{aligned} \tag{3.35}$$

the right-hand side containing the Gaussian fluctuation widths (3.24).

For the Coulomb potential (3.27) that we are interested in, the integral in the smearing formula (3.35) cannot be done exactly. An integral representation for a simple numerical treatment is

$$\begin{aligned}\left\langle-\frac{e^2}{4\pi\varepsilon_0|\mathbf{x}|}\right\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}&=-\frac{e^2}{4\pi\varepsilon_0}\sqrt{\frac{2}{\pi}a_\parallel^2(\mathbf{x}_0)}\int_0^1\frac{d\xi}{a_\parallel^2(\mathbf{x}_0)+\xi^2[a_\perp^2(\mathbf{x}_0)-a_\parallel^2(\mathbf{x}_0)]}\\&\quad\times\exp\left\{-\frac{\xi^2}{2}\left(\frac{x_0^2+y_0^2}{a_\parallel^2(\mathbf{x}_0)+\xi^2[a_\perp^2(\mathbf{x}_0)-a_\parallel^2(\mathbf{x}_0)]}+\frac{z_0^2}{a_\parallel^2(\mathbf{x}_0)}\right)\right\}.\end{aligned} \tag{3.36}$$

With this expression we know the entire first-order effective classical potential (3.23) for an electron in a Coulomb potential and a uniform magnetic field which has to be optimized in the variational parameters $\mathbf{\Omega}$.

IV. RESULTS

We are now going to optimize the effective classical potential by extremizing it in $\mathbf{\Omega}$ at different temperatures and magnetic-field strengths. In the zero-temperature limit this will produce the ground-state energy.

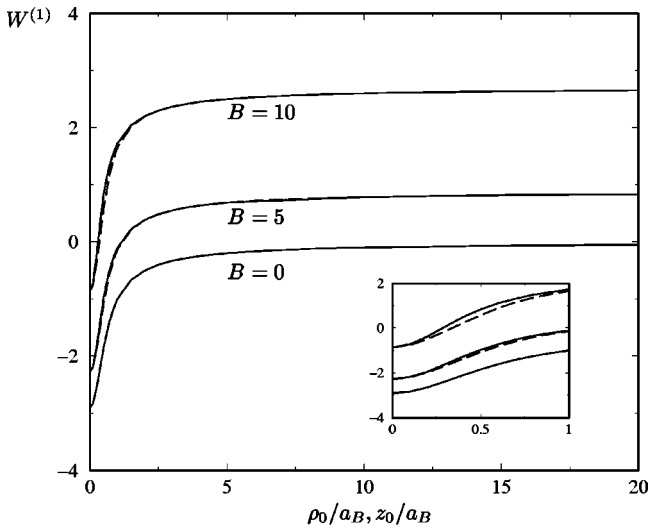

FIG. 1. Effective classical potential (in units of 2 Ry) as a function of the coordinate $\rho_0=\sqrt{x_0^2+y_0^2}$ perpendicular to the field lines at $z_0=0$ (solid curves), and parallel to the magnetic field as a function of z_0 at $\rho_0=0$ (dashed curves). The inverse temperature is fixed at $\beta=1$, and the strengths of the magnetic field B are varied (all in natural units). The small figure enlarges the range $0 \leqslant \rho_0, z_0 \leqslant 1$ with noticeable anisotropy.

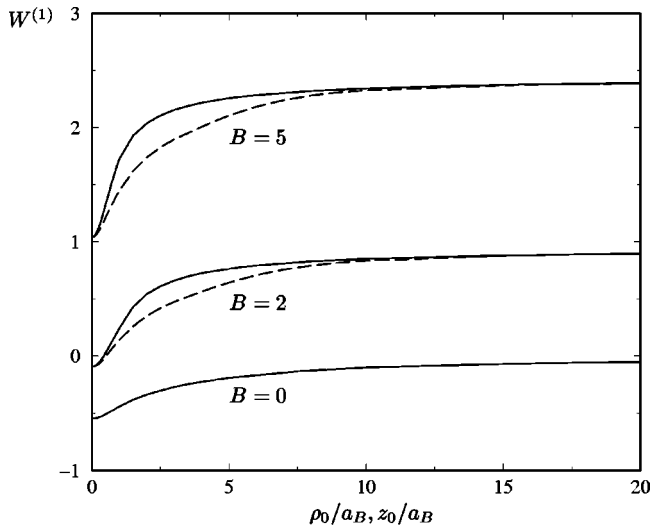

FIG. 2. Analogous plot to Fig. 1, but at the larger inverse temperature $\beta=100$.

A. Effective classical potential for different temperatures and magnetic field strengths

The optimization of $W_{\mathbf{\Omega}}^{(1)}(\mathbf{x}_0)$ proceeds by minimization in $\mathbf{\Omega}$ and must be done for each value of $\mathbf{x}_0$. Reinserting the optimal parameters $\mathbf{\Omega}^{(1)}(\mathbf{x}_0)$ into expressions (3.23) and (3.36), we obtain the optimal first-order effective classical potential $W^{(1)}(\mathbf{x}_0)$. The calculations are done numerically, where we used natural units $\hbar=e^2/4\pi\varepsilon_0=k_B=c=M=1$. This means that energies are measured in units of $\epsilon_0=Me^4/(4\pi\varepsilon_0)^2\hbar^2\equiv 2$ Ry≈ 27.21 eV, temperatures in $\epsilon_0/k_B\approx 3.16\times 10^5$ K, distances in Bohr radii $a_B=(4\pi\varepsilon_0)^2\hbar^2/Me^2\approx 0.53\times 10^{-10}$ m, and magnetic-field strengths in $B_0=e^3M^2/\hbar^3(4\pi\varepsilon_0)^2\approx 2.35\times 10^5$ T$=2.35\times 10^9$ G. Figure 1 shows the resulting curves for various magnetic-field strengths B and an inverse temperature $\beta=1/T=1$. Examples of the lower-temperature behavior are shown in Fig. 2 for $\beta=100$. To see the expected anisotropy of the curves in the magnetic-field direction and in the plane perpendicular to it, we simultaneously plot the curves for $W^{(1)}(\mathbf{x}_0)$ transversal to the magnetic field as a function of $\rho_0=\sqrt{x_0^2+y_0^2}$ at $z=0$ (solid curves) and parallel as a function of z_0 at $\rho_0=0$ (dashed curves). The curves become strongly anisotropic for low temperatures and increasing field strengths (Fig. 2). At a given field strength B, the two curves converge for large distances from the origin, where the proton resides, to the same constant depending on B. This is due to the decreasing influence of the Coulomb interaction which shows the classical $1/r$ behavior in each direction. When approaching the classical high-temperature limit, the effect of anisotropy becomes less important since the violent thermal fluctuations do not have a preferred direction (see Fig. 1). For $\rho_0\to\infty$ or $z_0\to\infty$, the expectation value of the Coulomb potential (3.36) tends to zero. The remaining effective classical potential

$$W_{\mathbf{\Omega}}^{(1)}(\mathbf{x}_0)\to -\frac{1}{\beta}\ln Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}-\Omega_B(\omega_B-\Omega_B)\,b_\perp^2 + (\omega_B^2-\Omega_\perp^2)\,a_\perp^2-\frac{1}{2}\Omega_\parallel^2 a_\parallel^2 \tag{4.1}$$

is a constant with regard to the position $\mathbf{x}_0$, and the optimization yields $\Omega_B^{(1)}=\Omega_\perp^{(1)}=\omega_B$ and $\Omega_\parallel^{(1)}=0$, leading to the asymptotic constant value

$$W^{(1)}(\mathbf{x}_0)\to -\frac{1}{\beta}\ln\frac{\beta\omega_B}{\sinh\beta\omega_B}. \tag{4.2}$$

The $B=0$ curves are of course identical with those obtained from variational perturbation theory for the hydrogen atom [20].

B. Ground-state energy of the hydrogen atom in uniform magnetic field

In what follows we investigate the zero-temperature behavior of the theory. Figures 1 and 2 show that the minimum of each potential curve lies at the origin. This means that the first-order approximation to the ground-state energy for a fixed magnitude of the magnetic field B is found by considering the zero-temperature limit of the first-order effective classical potential in the origin

$$E^{(1)}=\lim_{\beta\to\infty} W^{(1)}(0). \tag{4.3}$$

Thus we obtain from Eq. (3.23) the variational expression for the ground-state energy,

$$E_{\mathbf{\Omega}}^{(1)}(B)=\frac{1}{2\Omega_\perp}(\Omega_\perp^2+\omega_B^2)+\frac{\Omega_\parallel}{4}-\left\langle\frac{1}{|\mathbf{x}|}\right\rangle_{\mathbf{\Omega}}^{\mathbf{0}}, \tag{4.4}$$

where the expectation value for the Coulomb potential (3.36) can now be calculated exactly, since the exponential in the integral simplifies to unity:

$$\left\langle \frac{1}{|\mathbf{x}|} \right\rangle_{\mathbf{\Omega}}^{\mathbf{0}} = \sqrt{\frac{\Omega_\parallel}{\pi}} \frac{1}{\sqrt{1-\Omega_\parallel/\Omega_\perp}} \ln \frac{1-\sqrt{1-\Omega_\parallel/\Omega_\perp}}{1+\sqrt{1-\Omega_\parallel/\Omega_\perp}}. \tag{4.5}$$

Equations (4.4) and (4.5) are independent of the frequency parameter Ω_B such that the optimization of the first-order expression for the ground-state energy (4.4) requires satisfying the equations

$$\frac{\partial E_{\mathbf{\Omega}}^{(1)}(B)}{\partial \Omega_\perp} \stackrel{!}{=} 0, \quad \frac{\partial E_{\mathbf{\Omega}}^{(1)}(B)}{\partial \Omega_\parallel} \stackrel{!}{=} 0. \tag{4.6}$$

Reinserting the resulting values $\Omega_\perp^{(1)}$ and $\Omega_\parallel^{(1)}$ into Eq. (4.4) yields the first-order approximation for the ground-state energy $E^{(1)}(B)$. In the absence of the Coulomb interaction the optimization with respect to $\Omega_\perp$ yields $\Omega_\perp^{(1)}=\omega_B$, rendering the ground-state energy $E^{(1)}(B)=\omega_B$, which is the zeroth Landau level. An optimal value for $\Omega_\parallel$ does not exist since the dependence of the ground-state energy of this parameter is linear in Eq. (4.4) in this special case. To obtain the lowest energy, this parameter can be set to zero (all optimal frequency parameters used in the optimization procedure turn out to be nonnegative). For a vanishing magnetic field, $B=0$, Eq. (4.4) exactly reproduces the first-order variational result for the ground-state energy of the hydrogen atom, $E^{(1)}(B=0)\approx -0.42\,[2\,\mathrm{Ry}]$, obtained in Ref. [20].

To investigate the asymptotics in the strong-field limit $B\to\infty$, it is useful to extract the leading term ω_B. Thus we define the binding energy

$$\varepsilon(B)\equiv\omega_B - E(B), \tag{4.7}$$

which possesses a characteristic strong-field behavior to be discussed in detail subsequently. The result is shown in Fig. 3 as a function of the magnitude of the magnetic field B, where it is compared with the high-accuracy results of Ref. [1]. As a first-order approximation, this result is satisfactory. It is of the same quality as other first-order results, for example those from the operator optimization method in the first order of Ref. [5]. The advantage of variational perturbation theory is that it yields good results over the complete range of the coupling strength, here the magnetic field. Moreover, as a consequence of the exponential convergence (Ref. [17] Chap. 5), higher orders of variational perturbation theory push the approximate result of any quantity very rapidly toward the exact value.

1. Weak-field case

We now investigate the weak-field behavior of our theory, starting from expression (4.7) and the expectation value of the Coulomb potential (4.5) in natural units,

$$\varepsilon_{\eta,\Omega}^{(1)}(B) = \frac{B}{2} - \frac{\Omega}{2}\left(1+\frac{\eta}{2}\right) - \frac{B^2}{8\Omega} - \sqrt{\frac{\eta\Omega}{\pi}}\, h(\eta), \tag{4.8}$$

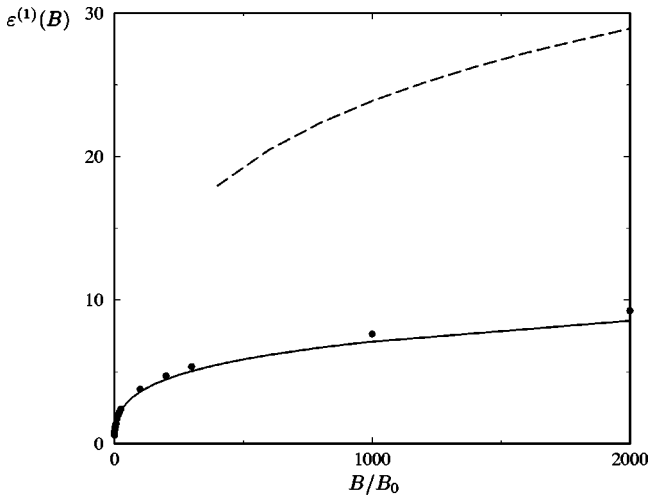

FIG. 3. First-order variational result for the binding energy (in units of 2 Ry) as a function of the strength of the magnetic field. The dots indicate the values of Ref. [1]. The dashed curve shows the simple estimate of Landau and Lifschitz [6] $0.5\ln^2 B$, which is closely related to the ground-state energy of the one-dimensional hydrogen atom [7,8].

with

$$h(\eta) = \frac{1}{\sqrt{1-\eta}} \ln \frac{1-\sqrt{1-\eta}}{1+\sqrt{1-\eta}}. \tag{4.9}$$

In comparison with Eq. (4.4), we introduce new variational parameters

$$\eta \equiv \frac{\Omega_\parallel}{\Omega_\perp}, \quad \Omega \equiv \Omega_\perp \tag{4.10}$$

and utilize, as calculations for the binding energy shown, that always $\eta \leqslant 1$. Performing the derivatives with respect to these variational parameters, and setting them equal to zero, yields conditional equations which, after some manipulations, can be written

$$\begin{aligned} &\frac{\Omega}{4} + \sqrt{\frac{\Omega}{\pi\eta}} \frac{1}{1-\eta}\left(1+\frac{1}{2}\frac{1}{\sqrt{1-\eta}} \ln \frac{1-\sqrt{1-\eta}}{1+\sqrt{1-\eta}}\right) \stackrel{!}{=} 0, \\ &\frac{1}{2} + \frac{\eta}{4} - \frac{B^2}{8\Omega^2} + \frac{1}{2}\sqrt{\frac{\eta}{\pi\Omega}} \frac{1}{\sqrt{1-\eta}} \ln \frac{1-\sqrt{1-\eta}}{1+\sqrt{1-\eta}} \stackrel{!}{=} 0. \end{aligned} \tag{4.11}$$

Expanding the variational parameters into perturbation series of the square magnetic field B^2,

$$\eta(B) = \sum_{n=0}^{\infty} \eta_n B^{2n}, \quad \Omega(B) = \sum_{n=0}^{\infty} \Omega_n B^{2n} \tag{4.12}$$

and inserting these expansions into the self-consistency conditions (4.11) we obtain order by order the coefficients given in Table I. Inserting these values into the expression for the binding energy (4.8) and expanding with respect to B^2, we obtain the perturbation series

TABLE I. Perturbation coefficients up to order B^6 for the weak-field expansions of the variational parameters and the binding energy in comparison to the exact ones of Ref. [2].

n	0	1	2	3
η_n	1.0	$-\frac{405\pi^2}{7168}\approx -0.5576$	$\frac{16828965\pi^4}{1258815488}\approx 1.3023$	$-\frac{3886999332075\pi^6}{884272562962432}\approx -4.2260$
Ω_n	$\frac{16}{9\pi}\approx 0.5659$	$\frac{99\pi}{448}\approx 0.6942$	$-\frac{1293975\pi^3}{39337984}\approx -1.0199$	$\frac{524431667187\pi^5}{55267035185152}\approx 2.9038$
ε_n	$-\frac{4}{3\pi}\approx -0.4244$	$\frac{9\pi}{128}\approx 0.2209$	$-\frac{8019\pi^3}{1835008}\approx -0.1355$	$\frac{256449807\pi^5}{322256764928}\approx 0.2435$
ε_n [2]	-0.5	0.25	$-\frac{53}{192}\approx -0.2760$	$\frac{5581}{4608}\approx 1.2112$

$$\varepsilon^{(1)}(B)=\frac{B}{2}-\sum_{n=0}^{\infty}\varepsilon_n B^{2n}. \tag{4.13}$$

The first coefficients are also given in Table I. We thus find the important result that the first-order variational perturbation solution possesses a perturbative behavior with respect to the square magnetic-field strength B^2 in the weak-field limit, thus yielding the correct asymptotics. The coefficients differ in higher order from the exact ones, but are improved in higher orders of the variational perturbation theory (Ref. [17] Chap. 5).

2. Asymptotical behavior in the strong-field regime

In the discussion of the pure magnetic field below Eq. (4.6), we mentioned that the variational calculation for the ground-state energy, which is thus associated with the zeroth Landau level, yields a frequency $\Omega_\perp \propto B$, while $\Omega_\parallel = 0$. Therefore, we use the assumption

$$\Omega_\perp \gg \Omega_\parallel, \quad \Omega_\parallel \ll B \tag{4.14}$$

for the consideration of the ground-state energy (4.4) of a hydrogen atom in a strong magnetic field. In a first step we expand the last expression of the expectation value (4.5) which corresponds to condition (4.14) in terms of $\Omega_\parallel/\Omega_\perp$ and reinsert this expansion into the equation of the ground-state energy (4.4). Then we omit all terms proportional to $C/\Omega_\perp$ where C stands for any expression with a value much smaller than the field strength B. In natural units, we thus obtain the strong-field approximation for the first-order binding energy (4.7):

$$\varepsilon^{(1)}_{\Omega_\perp,\Omega_\parallel}=\frac{B}{2}-\left(\frac{\Omega_\perp}{2}+\frac{B^2}{8\Omega_\perp}+\frac{\Omega_\parallel}{4}+\sqrt{\frac{\Omega_\parallel}{\pi}}\ln\frac{\Omega_\parallel}{4\Omega_\perp}\right). \tag{4.15}$$

As usual, we consider the zeros of the derivatives with respect to the variational parameters

$$\frac{\partial\varepsilon^{(1)}_{\Omega_\perp,\Omega_\parallel}}{\partial\Omega_\parallel}\overset{!}{=}0, \quad \frac{\partial\varepsilon^{(1)}_{\Omega_\perp,\Omega_\parallel}}{\partial\Omega_\perp}\overset{!}{=}0, \tag{4.16}$$

which lead to the self-consistence equations

$$\sqrt{\Omega_\parallel}\overset{!}{=}-\frac{2}{\sqrt{\pi}}(\ln\Omega_\parallel-\ln\Omega_\perp+2-\ln 4), \tag{4.17}$$

$$\Omega_\perp\overset{!}{=}\sqrt{\frac{\Omega_\parallel}{\pi}}+\frac{B}{2}\sqrt{1+4\frac{\Omega_\parallel}{\pi B^2}}. \tag{4.18}$$

Let us first consider the last equation. Utilizing the second of conditions (4.14), we expand the second root around unity, yielding the expression

$$\Omega_\perp=\frac{B}{2}+\sqrt{\frac{\Omega_\parallel}{\pi}}+\frac{\Omega_\parallel}{\pi B}-2\frac{\Omega_\parallel^2}{\pi^2B^3}+\cdots, \tag{4.19}$$

where the terms are sorted with regard to their contribution starting with the largest. Since we are interested in the strong-B limit, we can obviously neglect terms suppressed by powers of $1/B$. Thus we only consider the following terms for the moment:

$$\Omega_\perp\approx\frac{B}{2}+\sqrt{\frac{\Omega_\parallel}{\pi}}. \tag{4.20}$$

Inserting this into the other condition (4.17), expanding the corresponding logarithm, and, once again, neglecting terms of order $1/B$, we find

$$\sqrt{\Omega_\parallel}\approx\frac{2}{\sqrt{\pi}}(\ln B-\ln\Omega_\parallel+\ln 2-2). \tag{4.21}$$

To obtain a tractable approximation for $\Omega_\parallel$, we perform some iterations starting from

$$\sqrt{\Omega_\parallel^{(1)}}=\frac{2}{\sqrt{\pi}}\ln 2Be^{-2}. \tag{4.22}$$

Reinserting this on the right-hand side of Eq. (4.21), one obtains the second iteration $\sqrt{\Omega_\parallel^{(2)}}$. We stop this procedure after an additional reinsertion which yields

TABLE II. Example for the competing leading six terms in Eq. (4.29) at $B=10^5B_0\approx 2.35\times 10^{10}$ T.

$(1/\pi)\ln^2 B$	$-(4/\pi)\ln B\,\mathrm{lnln}\,B$	$(4/\pi)\,\ln^2\ln B$	$-(4b/\pi)\mathrm{lnln}\,B$	$[2(b+2)/\pi]\ln B$	b^2/π
42.1912	−35.8181	7.6019	4.8173	3.3098	0.7632

$$\sqrt{\Omega_\parallel^{(3)}}=\frac{2}{\sqrt{\pi}}\left(\ln 2Be^{-2}-2\ln\left[\frac{2}{\sqrt{\pi}}\left\{\ln 2Be^{-2}-2\ln\left(\frac{2}{\sqrt{\pi}}\ln 2Be^{-2}\right)\right\}\right]\right). \tag{4.23}$$

The reader may convince himself that this iteration procedure indeed converges. For a subsequent systematical extraction of terms essentially contributing to the binding energy, expression (4.23) is not satisfactory. Therefore, it is better to separate the leading term in the curly brackets and expand the logarithm of the remainder. Then this proceeding is applied to the expression in the angular brackets and so on. Neglecting terms of order $\ln^{-3}B$, we obtain

$$\sqrt{\Omega_\parallel^{(3)}}\approx\frac{2}{\sqrt{\pi}}\left(\ln 2Be^{-2}+\ln\frac{\pi}{4}-2\ln\ln 2Be^{-2}\right). \tag{4.24}$$

The double-logarithmic term can be expanded in a similar way as described above:

$$\begin{aligned}\mathrm{lnln}\,2Be^{-2}&=\ln\left[\ln B\left(1+\frac{\ln 2-2}{\ln B}\right)\right]\\&=\mathrm{lnln}\,B+\frac{\ln 2-2}{\ln B}-\frac{1}{2}\frac{(\ln 2-2)^2}{\ln^2 B}+O(\ln^{-3}B).\end{aligned} \tag{4.25}$$

Thus expression (4.24) may be rewritten as

$$\sqrt{\Omega_\parallel^{(3)}}=\frac{2}{\sqrt{\pi}}\left(\ln B-2\,\mathrm{lnln}\,B+\frac{2a}{\ln B}+\frac{a^2}{\ln^2 B}+b\right)+O(\ln^{-3}B), \tag{4.26}$$

with abbreviations

$$a=2-\ln 2\approx 1.307,\quad b=\ln\frac{\pi}{2}-2\approx -1.548. \tag{4.27}$$

The first observation is that the variational parameter $\Omega_\parallel$ is always much smaller than $\Omega_\perp$ in the high-B-field limit as has been assumed in (4.14). Thus we can further simplify approximation (4.20) by replacing

$$\Omega_\perp\approx\frac{B}{2}\left(1+\frac{2}{B}\sqrt{\frac{\Omega_\parallel}{\pi}}\right)\to\frac{B}{2}, \tag{4.28}$$

without affecting the following expression for the binding energy. Inserting solutions (4.26) and (4.28) into the equation for the binding energy (4.15), and expanding the logarithmic term once more as described, we find, up to the order $\ln^{-2}B$,

$$\begin{aligned}\varepsilon^{(1)}(B)=\frac{1}{\pi}\Bigg(&\ln^2 B-4\ln B\,\mathrm{lnln}\,B+4\ln^2\ln B-4b\,\mathrm{lnln}\,B\\&+2(b+2)\ln B+b^2-\frac{1}{\ln B}[8\ln^2\ln B-8b\,\mathrm{lnln}\,B\\&+2b^2]\Bigg)+O(\ln^{-2}B).\end{aligned} \tag{4.29}$$

Note that the prefactor $1/\pi$ of the leading $\ln^2 B$ term differs from a value 1/2 obtained by Landau and Lifschitz [6]. Our different value is a consequence of using a harmonic trial system. The calculation of higher orders in variational perturbation theory would improve the value of the prefactor.

At a magnetic-field strength $B=10^5B_0$, which corresponds to 2.35×10^{10} T, the contribution from the first six terms is 22.87[2 Ry]. The next three terms suppressed by a factor $\ln^{-1}B$ contribute −2.29[2 Ry], while an estimate for the $\ln^{-2}B$ terms yields nearly −0.3[2 Ry]. Thus we find

$$\varepsilon^{(1)}(10^5)=20.58\pm 0.3\,[2\ \mathrm{Ry}]. \tag{4.30}$$

This is in very good agreement with the value 20.60[2 Ry] obtained from the full treatment.

Table II lists the values of the first six terms of Eq. (4.29). This shows, in particular, the significance of the second leading term $-(4/\pi)\ln B\,\mathrm{lnln}\,B$, which is of the same order of the leading term $(1/\pi)\ln^2 B$ but with an opposite sign. In Fig. 3, we plot the expression

$$\varepsilon_L(B)=\frac{1}{2}\ln^2 B, \tag{4.31}$$

from Landau and Lifschitz [6], to illustrate that it gives far too large binding energies even at very large magnetic fields, e.g. at $2000B_0\propto 10^8$ T.

This strength of magnetic field appears on surfaces of neutron stars (10^6–10^8 T). A recently discovered type of neuton star is the so-called magnetar [22]. In these, charged particles such as protons and electrons produced by decaying neutrons give rise to the giant magnetic field of 10^{11} T. Magnetic fields of white dwarfs reach only up to 10^2–10^4 T. All these magnetic-field strengths are far from direct realization in experiments. The strongest magnetic fields ever produced in a laboratory were only of the order 10 T, an order of magnitude larger than the fields in sun spots, which reach about 0.4 T. Recall, for comparison, that the Earth's magnetic field has the small value of 0.6×10^{-4} T.

It should, however, be noted that there are systems in solid-state physics, where a rescaling of variables corresponds to extremly strong magnetic fields. In a donor-impured semiconductor like GaAs, the properties of the system of an electron bound to a positively charged donor nucleus in an external magnetic field of strength 6.57 T are comparable to a hydrogen atom in a field of strength 2.35×10^5 T [23]. The reason for this is the strongly reduced effective mass of the electron bound to the donor nucleus, the large dielectric constant of the semiconductor, and thus the much larger radius of the orbit of the electron. Hence the Coulomb interaction between the donor nucleus and the electron is much weaker than in the hydrogen atom. This approximate analogy between both systems can thus be used to investigate the effects of extremely strong magnetic fields in earthbound experiments.

As we see in Fig. 3, the nonleading terms in Eq. (4.29) give important contributions to the asymptotic behavior even at such large magnetic fields. It is an unusual property of the asymptotic behavior that the absolute value of the difference between the Landau expression (4.31) and our approximation (4.29) diverges with increasing magnetic-field strengths B; only the relative difference decreases.

V. SUMMARY

We have calculated the effective classical potential for the hydrogen atom in a magnetic field. For this we have generalized variational perturbation theory to make it applicable to physical systems with a uniform external magnetic field.

The effective classical potential containing the complete quantum statistical information of the system was determined in first-order variational perturbation theory. For zero temperature, it gave the energy of the system. Our result consists of a single analytic expression which is quite accurate at all temperatures and magnetic-field strengths.

ACKNOWLEDGMENTS

We thank Professor J. Čížek and Dr. J. Weniger for useful hints and references of a perturbative treatment of the ground-state properties of the hydrogen atom in a magnetic field. The authors also thank Dr. J. Ortner and M. Steinberg for discussions of the finite temperature behavior of this system. For interesting discussions we would also like to thank Professor J.T. Devreese and Professor G. Wunner. One of us (M.B.) is grateful for support from the Studienstiftung des deutschen Volkes.

APPENDIX A: GENERATING FUNCTIONAL FOR PARTICLE IN MAGNETIC FIELD AND HARMONIC-OSCILLATOR POTENTIAL

For the determination of the correlation functions of a system, we need to know the solution of the two-dimensional generating functional in the presence of an external source $\mathbf{j}=(j_x,j_y)$:

$$Z^{\mathbf{x}_0}[\mathbf{j}]=\lambda_{\rm th}^2\oint\mathcal{D}^2x\;\delta(\mathbf{x}_0-\overline{\mathbf{x}(\tau)})\,e^{-\mathcal{A}^{\mathbf{x}_0}[\mathbf{x};\mathbf{j}]/\hbar}. \tag{A1}$$

The action of a particle in a magnetic field in the z direction and a harmonic oscillator reads

$$\mathcal{A}^{\mathbf{x}_0}[\mathbf{x};\mathbf{j}]=\int_0^{\hbar\beta}d\tau\left[\frac{M}{2}\dot{\mathbf{x}}^2(\tau)-iM\Omega_B([\mathbf{x}(\tau)-\mathbf{x}_0]\times\dot{\mathbf{x}}(\tau))_z+\frac{1}{2}M(\Omega_\perp^2-\Omega_B^2)[\mathbf{x}(\tau)-\mathbf{x}_0]^2+\mathbf{j}(\tau)\cdot(\mathbf{x}(\tau)-\mathbf{x}_0)\right], \tag{A2}$$

where $\Omega_\perp>\Omega_B$, for stability. The position-dependent terms are centered around $\mathbf{x}_0=(x_0,y_0)$, which is the temporal average of the path $\mathbf{x}(\tau)$, and thus equal to the zero-frequency component of the Fourier path,

$$\mathbf{x}(\tau)=\mathbf{x}_0+\sum_{m=1}^{\infty}(\mathbf{x}_m e^{i\omega_m\tau}+\mathbf{x}_m^\star e^{-i\omega_m\tau}), \tag{A3}$$

with the Matsubara frequencies $\omega_m=2\pi m/\hbar\beta$ and complex Fourier coefficients $\mathbf{x}_m=\mathbf{x}_m^{\rm re}+i\mathbf{x}_m^{\rm im}$. Introducing a similar Fourier decomposition for the current $\mathbf{j}(\tau)$ with Fourier components $\mathbf{j}_m$ and using the orthonormality relation

$$\frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau\,e^{i(\omega_m-\omega_n)\tau}=\delta_{mn}, \tag{A4}$$

the generating functional can be written as

$$Z^{\mathbf{x}_0}[\mathbf{j}]=\prod_{m=1}^{\infty}\left[\int\frac{dx_m^{\rm re}dx_m^{\rm im}dy_m^{\rm re}dy_m^{\rm im}}{(\pi/M\beta\omega_m^2)^2}e^{-\mathcal{A}_m(\mathbf{x}_m,\mathbf{x}_m^\star;\mathbf{j}_m,\mathbf{j}_m^\star)/\hbar}\right], \tag{A5}$$

with

$$\begin{aligned}\mathcal{A}_m(\mathbf{x}_m,\mathbf{x}_m^\star;\mathbf{j}_m,\mathbf{j}_m^\star)=\hbar\beta M(\omega_m^2+\Omega_\perp^2-\Omega_B^2)([x_m^{\rm re}]^2+[x_m^{\rm im}]^2&\\+[y_m^{\rm re}]^2+[y_m^{\rm im}]^2)&\\+4i\hbar\beta M\Omega_B\omega_m(x_m^{\rm re}y_m^{\rm im}-x_m^{\rm im}y_m^{\rm re})&\\+2\hbar\beta(x_m^{\rm re}j_{xm}^{\rm re}+x_m^{\rm im}j_{xm}^{\rm im}+y_m^{\rm re}j_{ym}^{\rm re}&\\+y_m^{\rm im}j_{ym}^{\rm im}).&\end{aligned} \tag{A6}$$

Expression (A5) is equivalent to the path integral (A1) and after performing integrations and retransforming the currents

$$\mathbf{j}_m=\frac{1}{\hbar\beta}\int_0^{\hbar\beta}d\tau\,\mathbf{j}(\tau)e^{-i\omega_m\tau}, \tag{A7}$$

we obtain the resulting generating functional

$$Z^{\mathbf{x}_0}[\mathbf{j}]=Z^{\mathbf{x}_0}\exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\;\mathbf{j}(\tau)\mathbf{G}^{\mathbf{x}_0}(\tau,\tau')\mathbf{j}(\tau')\right\}, \tag{A8}$$

with the partition function

$$Z^{\mathbf{x}_0} \equiv Z^{\mathbf{x}_0}[0] = \prod_{m=1}^{\infty} \frac{\omega_m^4}{4\Omega_B^2\omega_m^2 + (\omega_m^2 + \Omega_\perp^2)^2}, \tag{A9}$$

and the 2×2 matrix of the Green functions:

$$\mathbf{G}^{\mathbf{x}_0}(\tau,\tau') = \begin{pmatrix} G_{xx}^{\mathbf{x}_0}(\tau,\tau') & G_{xy}^{\mathbf{x}_0}(\tau,\tau') \\ G_{yx}^{\mathbf{x}_0}(\tau,\tau') & G_{yy}^{\mathbf{x}_0}(\tau,\tau') \end{pmatrix}. \tag{A10}$$

The elements of this matrix are position-position correlation functions what can be easily proved by applying two functional derivatives with respect to the desired component of the current to functional (A1), for example,

$$G_{xx}^{\mathbf{x}_0}(\tau,\tau') = \langle (x(\tau)-x_0)\,(x(\tau')-x_0)\rangle^{\mathbf{x}_0} = \left[\hbar^2 \frac{1}{Z^{\mathbf{x}_0}[\mathbf{j}]} \frac{\delta^2}{\delta j_x(\tau)\,\delta j_x(\tau')} Z^{\mathbf{x}_0}[\mathbf{j}]\right]_{\mathbf{j}=0}, \tag{A11}$$

where we have defined expectation values by

$$\langle \cdots \rangle^{\mathbf{x}_0} = \frac{\lambda_{\rm th}^2}{Z^{\mathbf{x}_0}} \oint \mathcal{D}^2 x \ \ldots\ \delta(\mathbf{x}_0 - \overline{\mathbf{x}(\tau)}) e^{-\mathcal{A}^{\mathbf{x}_0}[\mathbf{x};0]/\hbar}. \tag{A12}$$

From the above calculation, we find the following expressions for the Green functions in Fourier space ($0 \leqslant \tau,\tau' \leqslant \hbar\beta$):

$$G_{xx}^{\mathbf{x}_0}(\tau,\tau') = \langle \tilde{x}(\tau)\,\tilde{x}(\tau')\rangle^{\mathbf{x}_0} = G_{yy}^{\mathbf{x}_0}(\tau,\tau') = \langle \tilde{y}(\tau)\,\tilde{y}(\tau')\rangle^{\mathbf{x}_0} = \frac{2}{M\beta} \sum_{m=1}^{\infty} \frac{\omega_m^2 + \Omega_\perp^2 - \Omega_B^2}{4\Omega_B^2\omega_m^2 + (\omega_m^2 + \Omega_\perp^2 - \Omega_B^2)^2} \times e^{-i\omega_m(\tau-\tau')}, \tag{A13}$$

$$G_{xy}^{\mathbf{x}_0}(\tau,\tau') = \langle \tilde{x}(\tau)\,\tilde{y}(\tau')\rangle^{\mathbf{x}_0} = -G_{yx}^{\mathbf{x}_0}(\tau,\tau') = -\langle \tilde{y}(\tau)\,\tilde{x}(\tau')\rangle^{\mathbf{x}_0} = \frac{4\Omega_B}{M\beta} \sum_{m=1}^{\infty} \frac{\omega_m}{4\Omega_B^2\omega_m^2 + (\omega_m^2 + \Omega_\perp^2 - \Omega_B^2)^2} \times e^{-i\omega_m(\tau-\tau')}, \tag{A14}$$

where, for simplicity, $\tilde{\mathbf{x}}(\tau) = \mathbf{x}(\tau) - \mathbf{x}_0$. It is desirable to find analytical expressions for the Green functions and the partition function (A9). All these quantities possess the same denominator, which can be decomposed as

$$4\Omega_B^2\omega_m^2 + (\omega_m^2 + \Omega_\perp^2 - \Omega_B^2)^2 = (\omega_m^2 + \Omega_+^2)(\omega_m^2 + \Omega_-^2) \tag{A15}$$

with frequencies

$$\Omega_\pm(\Omega_B,\Omega_\perp) = \Omega_\perp \pm \Omega_B. \tag{A16}$$

Therefore the partition function (A9) can be split into two products, each of which known from the harmonic oscillator (Ref. [17] Chap. 5):

$$Z^{\mathbf{x}_0} = \prod_{m=1}^{\infty} \left[\frac{\omega_m^2}{\omega_m^2 + \Omega_+^2}\right] \prod_{m=1}^{\infty} \left[\frac{\omega_m^2}{\omega_m^2 + \Omega_-^2}\right] = \frac{\hbar\beta\Omega_+/2}{\sinh \hbar\beta\Omega_+/2} \frac{\hbar\beta\Omega_-/2}{\sinh \hbar\beta\Omega_-/2}. \tag{A17}$$

Now we apply property (A15) to decompose the Green function (A13) into partial fractions, yielding

$$G_{xx}^{\mathbf{x}_0}(\tau,\tau') = G_{yy}^{\mathbf{x}_0}(\tau,\tau') = \frac{1}{M\beta}\left(\alpha_1 \sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + \Omega_+^2} e^{-i\omega_m(\tau-\tau')} + \alpha_2 \sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + \Omega_-^2} e^{-i\omega_m(\tau-\tau')} - \frac{1}{\Omega_+\Omega_-}\right), \tag{A18}$$

with coefficients

$$\alpha_1 = \frac{\Omega_+^2 - \Omega_\perp^2 + \Omega_B^2}{\Omega_+^2 - \Omega_-^2} = \frac{\Omega_\perp + \Omega_B}{2\Omega_\perp},$$

$$\alpha_2 = -\frac{\Omega_-^2 - \Omega_\perp^2 + \Omega_B^2}{\Omega_+^2 - \Omega_-^2} = \frac{\Omega_\perp - \Omega_B}{2\Omega_\perp}. \tag{A19}$$

Following Ref. [17] Chap. 3, sums of the kind occuring in expression (A18) are spectral decompositions of the correlation function for the harmonic oscillator, and can be summed up as

$$\sum_{m=-\infty}^{\infty} \frac{1}{\omega_m^2 + \Omega_\pm^2} e^{-i\omega_m(\tau-\tau')} = \frac{\hbar\beta}{2\Omega_\pm} g_\pm(\tau,\tau'). \tag{A20}$$

Here we introduced the expression

$$g_\varepsilon(\tau,\tau') = \frac{\cosh \Omega_\varepsilon(|\tau-\tau'| - \hbar\beta/2)}{\sinh \hbar\beta\Omega_\varepsilon/2}, \quad \tau,\tau' \in (0,\hbar\beta), \tag{A21}$$

with $\varepsilon \in \{+,-,\perp,\|\}$. Thus, the xx and yy correlation functions can be expressed by

$$G_{xx}^{\mathbf{x}_0}(\tau,\tau') = G_{yy}^{\mathbf{x}_0}(\tau,\tau') = \frac{1}{M\beta}\left(\frac{\hbar\beta}{4\Omega_\perp} g_+(\tau,\tau') + \frac{\hbar\beta}{4\Omega_\perp} g_-(\tau,\tau') - \frac{1}{\Omega_+\Omega_-}\right), \tag{A22}$$

where, from Eq. (A16), $\Omega_\pm = \Omega_\pm(\Omega_B,\Omega_\perp)$ are functions of the original frequencies Ω_B from the magnetic field and $\Omega_\perp$ from the additional harmonic oscillator (A2). It is ob-

vious that expression (A22) reduces to the Green function of the harmonic oscillator for $\Omega_B \to 0$,

$$\lim_{\Omega_B\to 0} G_{ii}^{\mathbf{x}_0}(\tau,\tau') = \frac{1}{M\beta\Omega_\perp^2}\left(\frac{\hbar\beta\Omega_\perp}{2} g_\perp(\tau,\tau') - 1\right), \tag{A23}$$

with $i \in \{x,y\}$. In this limit, partition function (A17) turns out to be the usual one (Ref. [17] Chap. 5) for such a harmonic oscillator:

$$\lim_{\Omega_B\to 0} Z^{\mathbf{x}_0} = \frac{\hbar\beta\Omega_\perp/2}{\sinh \hbar\beta\Omega_\perp/2}. \tag{A24}$$

It is worth mentioning that with the last term in Green function (A22), the classical harmonic fluctuation width

$$G_{xx}^{\mathrm{cl}} = \langle x^2\rangle^{\mathrm{cl}} = \frac{1}{M\beta(\Omega_\perp^2 - \Omega_B^2)} \tag{A25}$$

is subtracted. This is the consequence of the exclusion of the zero frequency mode of the Fourier path (A3) in the generating functional (A1). The necessity to do this was already discussed in Sec. II. The other terms in Eq. (A22) are those which we would have obtained *without* separation of the $\mathbf{x}_0$ component. Thus these terms represent the quantum-mechanical Green function containing all quantum fluctuations as well as thermal fluctuations. It is a nice property of all Green functions discussed in this paper that

$$G_{xx}^{\mathbf{x}_0}(\tau,\tau') = G_{xx}^{\mathrm{qm}}(\tau,\tau') - G_{xx}^{\mathrm{cl}}. \tag{A26}$$

Such a relation exists for all other Green functions appropriately, including momentum-position correlations which we consider subsequently.

The knowledge of relation (A20) makes it quite easy to determine the algebraic expression for the mixed xy correlation functions. Rewriting Eq. (A14) as

$$\begin{aligned} G_{xy}^{\mathbf{x}_0}(\tau,\tau') &= -G_{yx}^{\mathbf{x}_0}(\tau,\tau') \\ &= \frac{i}{2M\beta\Omega_\perp}\frac{\partial}{\partial\tau}\left(\sum_{m=-\infty}^{\infty}\frac{1}{\omega_m^2+\Omega_+^2}e^{-i\omega_m(\tau-\tau')}\right. \\ &\quad \left. + \sum_{m=-\infty}^{\infty}\frac{1}{\omega_m^2+\Omega_-^2}e^{-i\omega_m(\tau-\tau')}\right), \end{aligned} \tag{A27}$$

and applying the derivative with respect to τ to relation (A20), we obtain the following expression for the mixed Green function:

$$\begin{aligned} G_{xy}^{\mathbf{x}_0}(\tau,\tau') = -G_{yx}^{\mathbf{x}_0}(\tau,\tau') &= \frac{\hbar}{4iM\Omega_\perp}\{\Theta(\tau-\tau')[h_+(\tau,\tau') \\ &\quad - h_-(\tau,\tau')] - \Theta(\tau'-\tau)[h_+(\tau',\tau) \\ &\quad - h_-(\tau',\tau)]\}, \end{aligned} \tag{A28}$$

where we have used the abbreviation

$$h_\varepsilon(\tau,\tau') = \frac{\sinh\Omega_\varepsilon(\tau-\tau'-\hbar\beta/2)}{\sinh\hbar\beta\Omega_\varepsilon/2}, \quad \tau,\tau' \in (0,\hbar\beta), \tag{A29}$$

with $\varepsilon \in \{+,-,\perp,\|\}$. Note that classically $\langle xy\rangle^{\mathrm{cl}} = 0$, such that Eq. (A26) reduces to

$$G_{xy}^{\mathbf{x}_0}(\tau,\tau') = G_{xy}^{\mathrm{qm}}(\tau,\tau'). \tag{A30}$$

The Heaviside function in Eq. (A28) is defined symmetrically:

$$\Theta(\tau-\tau') = \begin{cases} 1, & \tau > \tau' \\ 1/2, & \tau = \tau' \\ 0, & \tau < \tau'. \end{cases} \tag{A31}$$

In the quantum-mechanical limit of zero temperature ($\beta \to \infty$), the Green function (A22) simplifies to

$$\begin{aligned} \lim_{\beta\to\infty} G_{xx}^{\mathbf{x}_0}(\tau,\tau') &= \lim_{\beta\to\infty} G_{yy}^{\mathbf{x}_0}(\tau,\tau') \\ &= \frac{\hbar}{4M\Omega_\perp}(e^{-\Omega_+|\tau-\tau'|} + e^{-\Omega_-|\tau-\tau'|}), \end{aligned} \tag{A32}$$

while in Eq. (A28) only $h_\pm(\tau,\tau')$ changes:

$$\lim_{\beta\to\infty} h_\pm(\tau,\tau') = -e^{-\Omega_\pm(\tau-\tau')}. \tag{A33}$$

APPENDIX B: PROPERTIES OF GREEN FUNCTIONS

In this section we list properties of Green functions (A22) and (A28), which are important for the forthcoming consideration of the generating functional with sources coupling linearily to position or momentum in Appendix C. For all relations, we suppose that $0 \leqslant \tau,\tau' \leqslant \hbar\beta$.

1. General properties

A first observation is the temporal translational invariance of the Green function,

$$G_{ij}^{\mathbf{x}_0}(\tau,\tau') = G_{ij}^{\mathbf{x}_0}(\tau-\tau'), \tag{B1}$$

where each of the indices i and j stands for x or y, respectively. For equal times we find

$$G_{ij}^{\mathbf{x}_0}(\tau,\tau) = \frac{1}{M\beta}\left(\frac{\hbar\beta}{4\Omega_\perp}g_+(\tau,\tau) + \frac{\hbar\beta}{4\Omega_\perp}g_-(\tau,\tau) - \frac{1}{\Omega_+\Omega_-}\right) \times \begin{cases} 1, & i=j \\ 0, & i\neq j. \end{cases} \tag{B2}$$

Moreover we read off the following symmetries from expressions (A22) and (A28):

$$G_{ij}^{\mathbf{x}_0}(\tau,\tau') = G_{ij}^{\mathbf{x}_0}(\tau',\tau) \times \begin{cases} 1, & i=j \\ -1, & i\neq j. \end{cases} \tag{B3}$$

Otherwise,

$$G_{ij}^{\mathbf{x}_0}(\tau,\tau') = G_{ji}^{\mathbf{x}_0}(\tau',\tau). \tag{B4}$$

Throughout the paper we always use periodic paths. Hence it is obvious that all Green functions are also periodic:

$$G_{ij}^{\mathbf{x}_0}(0,\tau') = G_{ij}^{\mathbf{x}_0}(\hbar\beta,\tau'), \quad G_{ij}^{\mathbf{x}_0}(\tau,0) = G_{ij}^{\mathbf{x}_0}(\tau,\hbar\beta). \tag{B5}$$

2. Derivatives of Green functions

We now proceed with derivatives of the Green functions (A22) and (A28), since these are essential for the derivation of the generating functional of position- and momentum-dependent correlations in Appendix C.

Before considering concrete expressions, we introduce a new symbol indicating uniquely to which argument the derivative is applied. A dot on the left-hand side means to perform the derivative with respect to the first argument and the dot on the right-hand side indicates that to differentiate with respect to the other argument. Having a dot on both sides, the Green function is derived with respect to both arguments:

$$\dot{G}_{ij}^{\mathbf{x}_0}(\tau,\tau') = \frac{\partial G_{ij}^{\mathbf{x}_0}(\tau,\tau')}{\partial\tau},$$

$$G'^{\mathbf{x}_0}_{ij}(\tau,\tau') = \frac{\partial G_{ij}^{\mathbf{x}_0}(\tau,\tau')}{\partial\tau'},$$

$$\dot{G}'^{\mathbf{x}_0}_{ij}(\tau,\tau') = \frac{\partial^2 G_{ij}^{\mathbf{x}_0}(\tau,\tau')}{\partial\tau\partial\tau'}. \tag{B6}$$

Applying such derivatives to Green functions (A22), we obtain ($i \in \{x,y\}$)

$$\begin{aligned}\dot{G}_{ii}^{\mathbf{x}_0}(\tau,\tau') &= \frac{\hbar}{4M\Omega_\perp}[\Theta(\tau-\tau')f_1(\tau,\tau') \\ &\quad -\Theta(\tau'-\tau)f_1(\tau',\tau)] \\ &= -G'^{\mathbf{x}_0}_{ii}(\tau,\tau'),\end{aligned} \tag{B7}$$

with

$$f_1(\tau,\tau') = (\Omega_\perp+\Omega_B)h_+(\tau,\tau') + (\Omega_\perp-\Omega_B)h_-(\tau,\tau'), \tag{B8}$$

where $h_\pm(\tau,\tau)$ was defined in Eq. (A29). Performing the derivatives to both arguments leads to the expression

$$\dot{G}'^{\mathbf{x}_0}_{ii}(\tau,\tau') = \dot{\tilde{G}}'^{\mathbf{x}_0}_{ii}(\tau,\tau') + \frac{\hbar}{M}\delta(\tau-\tau'), \tag{B9}$$

where we have introduced the partial function

$$\dot{\tilde{G}}'^{\mathbf{x}_0}_{ii}(\tau,\tau') = -\frac{\hbar}{4M\Omega_\perp}[\Omega_+^2 g_+(\tau,\tau') + \Omega_-^2 g_-(\tau,\tau')], \tag{B10}$$

which is finite for equal times.

Applying derivatives with respect to the first respective second argument to the mixed correlation function (A28), we find

$$\begin{aligned}\dot{G}_{xy}^{\mathbf{x}_0}(\tau,\tau') &= \frac{\hbar}{4iM\Omega_\perp}[\Omega_+ g_+(\tau,\tau') - \Omega_- g_-(\tau,\tau')] \\ &= -G'^{\mathbf{x}_0}_{xy}(\tau,\tau')\end{aligned} \tag{B11}$$

and

$$\dot{G}_{yx}^{\mathbf{x}_0}(\tau,\tau') = -\dot{G}_{xy}^{\mathbf{x}_0}(\tau,\tau'). \tag{B12}$$

Differentiating each argument of the mixed Green function results in

$$\begin{aligned}\dot{G}'^{\mathbf{x}_0}_{xy}(\tau,\tau') &= \frac{i\hbar}{4M\Omega_\perp}[\Theta(\tau-\tau')f_2(\tau,\tau') \\ &\quad -\Theta(\tau'-\tau)f_2(\tau',\tau)] \\ &= -\dot{G}'^{\mathbf{x}_0}_{yx}(\tau,\tau').\end{aligned} \tag{B13}$$

with

$$f_2(\tau,\tau') = (\Omega_\perp+\Omega_B)^2 h_+(\tau,\tau') - (\Omega_\perp-\Omega_B)^2 h_-(\tau,\tau'). \tag{B14}$$

An additional property we read off from Eqs. (B7) and (B11) is ($i,j \in \{x,y\}$):

$$\dot{G}_{ij}^{\mathbf{x}_0}(\tau,\tau') = \dot{G}_{ij}^{\mathbf{x}_0}(\tau',\tau)\times\begin{cases}-1, & i=j\\ 1, & i\neq j,\end{cases} \tag{B15}$$

$$G'^{\mathbf{x}_0}_{ij}(\tau,\tau') = G'^{\mathbf{x}_0}_{ij}(\tau',\tau)\times\begin{cases}-1, & i=j\\ 1, & i\neq j.\end{cases} \tag{B16}$$

The double-sided derivatives (B9), (B10), and (B13) imply

$$\dot{G}'^{\mathbf{x}_0}_{ij}(\tau,\tau') = \dot{G}'^{\mathbf{x}_0}_{ij}(\tau',\tau)\times\begin{cases}1, & i=j\\ -1, & i\neq j.\end{cases} \tag{B17}$$

Derivatives (B7), (B10), (B11), and (B13) are periodic:

$$\dot{G}_{ij}^{\mathbf{x}_0}(\tau,0) = \dot{G}_{ij}^{\mathbf{x}_0}(\tau,\hbar\beta), \quad \dot{G}_{ij}^{\mathbf{x}_0}(0,\tau') = \dot{G}_{ij}^{\mathbf{x}_0}(\hbar\beta,\tau'), \tag{B18}$$

$$G'^{\mathbf{x}_0}_{ij}(\tau,0) = G'^{\mathbf{x}_0}_{ij}(\tau,\hbar\beta), \quad G'^{\mathbf{x}_0}_{ij}(0,\tau') = G'^{\mathbf{x}_0}_{ij}(\hbar\beta,\tau'), \tag{B19}$$

$$\begin{aligned}\dot{\tilde{G}}'^{\mathbf{x}_0}_{ii}(\tau,0) &= \dot{\tilde{G}}'^{\mathbf{x}_0}_{ii}(\tau,\hbar\beta), \\ \dot{\tilde{G}}'^{\mathbf{x}_0}_{ii}(0,\tau') &= \dot{\tilde{G}}'^{\mathbf{x}_0}_{ii}(\hbar\beta,\tau'), \\ \dot{G}'^{\mathbf{x}_0}_{ij}(\tau,0) &= \dot{G}'^{\mathbf{x}_0}_{ij}(\tau,\hbar\beta),\end{aligned} \tag{B20}$$

$$\overset{\bullet}{G}{}^{\mathbf{x}_0}_{ij}(0,\tau') = \overset{\bullet}{G}{}^{\mathbf{x}_0}_{ij}(\hbar\beta,\tau') \quad (i \neq j). \tag{B21}$$

APPENDIX C: GENERATING FUNCTIONAL FOR POSITION- AND MOMENTUM-DEPENDENT CORRELATION FUNCTIONS

With the discussion of the generating functional for position-dependent correlation functions and, in particular, the Green functions in Appendix A, and that of their properties in Appendix B, we have laid the foundation to derive a generating functional for correlation functions depending on both position and momentum. Following the framework presented in an earlier work [21], such a functional involving sources coupled to the momentum can always be reduced to one containing position-coupled sources only.

We start from a three-dimensional effective classical representation for the generating functional

$$Z_{\mathbf{\Omega}}[\mathbf{j},\mathbf{v}] = \int \frac{d^3x_0 d^3p_0}{(2\pi\hbar)^3} Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j},\mathbf{v}], \tag{C1}$$

with zero-frequency components $\mathbf{x}_0 = (x_0, y_0, z_0) = \text{const}$ and $\mathbf{p}_0 = (p_{x0}, p_{y0}, p_{y0}) = \text{const}$ of the Fourier path separated. The reduced functional is

$$Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j},\mathbf{v}] = (2\pi\hbar)^3 \oint \mathcal{D}'^3x \mathcal{D}^3p \; \delta(\mathbf{x}_0 - \overline{\mathbf{x}(\tau)}) \times \delta(\mathbf{p}_0 - \overline{\mathbf{p}(\tau)}) \exp\left\{ -\frac{1}{\hbar} \mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x};\mathbf{j},\mathbf{v}] \right\}, \tag{C2}$$

where the path integral measure is that defined in Eq. (2.4). Extending action (2.3) by source terms, considering a more general Hamilton function than Eq. (2.18), and introducing an additional harmonic oscillator in the z direction, the action functional in Eq. (C2) reads

$$\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{p},\mathbf{x};\mathbf{j},\mathbf{v}] = \int_0^{\hbar\beta} d\tau \left\{ -i\tilde{\mathbf{p}}(\tau)\cdot\dot{\mathbf{x}}(\tau) + \frac{1}{2M}\tilde{\mathbf{p}}^2(\tau) - \Omega_B l_z(\tilde{\mathbf{p}},\tilde{\mathbf{x}}) + \frac{1}{2}M\Omega_\perp^2[\tilde{x}^2(\tau)+\tilde{y}^2(\tau)] + \frac{1}{2}M\Omega_\parallel^2\tilde{z}^2(\tau) + \mathbf{j}(\tau)\cdot\tilde{\mathbf{x}}(\tau) + \mathbf{v}(\tau)\cdot\tilde{\mathbf{p}}(\tau) \right\} \tag{C3}$$

with shifted positions and momenta

$$\tilde{\mathbf{x}} = \mathbf{x}(\tau) - \mathbf{x}_0, \quad \tilde{\mathbf{p}} = \mathbf{p}(\tau) - \mathbf{p}_0. \tag{C4}$$

The orbital angular momentum $l_z(\mathbf{p},\mathbf{x})$ is defined in Eq. (2.19), and used in Eq. (C3) with shifted phase-space coordinates (C4). We have introduced three different frequencies in Eq. (C3), $\mathbf{\Omega} = (\Omega_B, \Omega_\perp, \Omega_\parallel)$, where the first both components are used in regard to the oscillations in the plane perpendicular to the direction of the magnetic field which shall be considered here to point in the z direction. The last component $\Omega_\parallel$ is the frequency of a trial oscillator parallel to the field lines.

Due to the periodicity of the paths, we suppose that the sources might also be periodic:

$$\mathbf{j}(0) = \mathbf{j}(\hbar\beta), \quad \mathbf{v}(0) = \mathbf{v}(\hbar\beta). \tag{C5}$$

Since we want to simplify expression (C2), such that we can use the results obtained in Appendix A, the momentum path integral is solved in the following. In a first step we reexpress the momentum δ function in Eq. (C2) by

$$\delta(\mathbf{p}_0 - \overline{\mathbf{p}(\tau)}) = \int \frac{d^3\xi}{(2\pi\hbar)^3} \exp\left\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\, \mathbf{v}_0\cdot[\mathbf{p}(\tau) - \mathbf{p}_0] \right\}, \tag{C6}$$

where

$$\mathbf{v}_0(\boldsymbol{\xi}) = \frac{i}{\hbar\beta}\boldsymbol{\xi} \tag{C7}$$

is an additional current which is coupled to the momentum and is constant in time. Defining the sum of all sources coupled to the momentum by

$$\mathbf{V}(\boldsymbol{\xi},\tau) = \mathbf{v}(\tau) + \mathbf{v}_0(\boldsymbol{\xi}), \tag{C8}$$

functional (C2) can be written as

$$Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j},\mathbf{v}] = \int d^3\xi \oint \mathcal{D}'^3x \mathcal{D}^3p \; \delta(\mathbf{x}_0 - \overline{\mathbf{x}(\tau)}) \times \exp\left\{ -\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \left[-i\mathbf{p}(\tau)\cdot\dot{\mathbf{x}}(\tau) + \frac{\mathbf{p}^2(\tau)}{2M} - \Omega_B l_z(\mathbf{p}(\tau),\tilde{\mathbf{x}}(\tau)) + \frac{1}{2}M\Omega_\perp^2\{\tilde{x}^2(\tau)+\tilde{y}^2(\tau)\} + \frac{1}{2}M\Omega_\parallel^2\tilde{z}^2(\tau) + \mathbf{j}(\tau)\cdot\tilde{\mathbf{x}}(\tau) + \mathbf{V}(\boldsymbol{\xi},\tau)\cdot\mathbf{p}(\tau) \right] \right\}, \tag{C9}$$

where we have used the translation invariance $\tilde{\mathbf{p}} \to \mathbf{p}$ of the path integral. To solve the momentum path integral, it is useful to express it in its discretized form. Performing quadratic completions such that the momentum path integral separates into an infinite product of simple Gaussian integrals which are easily calculated, the remaining functional is reduced to the configuration space path integral

$$Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j},\mathbf{v}] = \int d^3\xi \exp\left[\frac{M}{2\hbar}\int_0^{\hbar\beta} d\tau\, \mathbf{V}^2(\boldsymbol{\xi},\tau) \right] \oint \mathcal{D}^3x \times \delta(\mathbf{x}_0 - \overline{\mathbf{x}(\tau)}) \exp\left\{ -\frac{1}{\hbar}\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{x};\mathbf{j},\mathbf{V}] \right\} \tag{C10}$$

with the measure (2.10) for $D=3$. The action functional is

$$\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{x};\mathbf{j},\mathbf{V}]=\int_0^{\hbar\beta}d\tau\left[\frac{M}{2}\dot{\mathbf{x}}^2(\tau)+iM\Omega_B\{\dot{x}(\tau)\tilde{y}(\tau)-\dot{y}(\tau)\tilde{x}(\tau)\}+\frac{1}{2}M(\Omega_\perp^2-\Omega_B^2)\{\tilde{x}^2(\tau)+\tilde{y}^2(\tau)\}+\frac{1}{2}M\Omega_\parallel^2\tilde{z}^2(\tau)+\tilde{x}(\tau)[j_x(\tau)+M\Omega_B V_y(\boldsymbol{\xi},\tau)]+\tilde{y}(\tau)[j_y(\tau)-M\Omega_B V_x(\boldsymbol{\xi},\tau)]+\tilde{z}(\tau)j_z(\tau)\right]-\frac{iM}{\hbar}\int_0^{\hbar\beta}d\tau\,\dot{\mathbf{x}}(\tau)\cdot\mathbf{V}(\boldsymbol{\xi},\tau),\tag{C11}$$

where the last term simplifies by the following consideration. A partial integration of this term yields

$$\int_0^{\hbar\beta}d\tau\,\dot{\mathbf{x}}(\tau)\cdot\mathbf{V}(\boldsymbol{\xi},\tau)=-\int_0^{\hbar\beta}d\tau\,(\mathbf{x}(\tau)-\mathbf{x}_0)\cdot\dot{\mathbf{V}}(\boldsymbol{\xi},\tau).\tag{C12}$$

The surface term vanishes as a consequence of the periodicity of the path and the source. This periodicity is also the reason why we could shift $\mathbf{x}(\tau)$ by the constant $\mathbf{x}_0$ on the right-hand side of Eq. (C12). Obviously, the importance of this expression lies in the coupling of the time derivative of $\mathbf{V}(\boldsymbol{\xi},\tau)$ to the path $\mathbf{x}(\tau)$. Thus $\dot{\mathbf{V}}(\boldsymbol{\xi},\tau)$ can be handled like a $\mathbf{j}(\tau)$ current [21], the action (C11) can be written as

$$\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{x};\mathbf{j},\mathbf{V}]=\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{x};\mathbf{J},0]=\mathcal{A}_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{x};0,0]-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\,\tilde{\mathbf{x}}(\tau)\cdot\mathbf{J}(\boldsymbol{\xi},\tau),\tag{C13}$$

with a new current vector $\mathbf{J}(\boldsymbol{\xi},\tau)$ which has the components

$$\begin{aligned}J_x(\boldsymbol{\xi},\tau)&=j_x(\tau)+M\Omega_B V_y(\boldsymbol{\xi},\tau)-iM\dot{V}_x(\boldsymbol{\xi},\tau),\\ J_y(\boldsymbol{\xi},\tau)&=j_y(\tau)-M\Omega_B V_x(\boldsymbol{\xi},\tau)-iM\dot{V}_y(\boldsymbol{\xi},\tau),\\ J_z(\boldsymbol{\xi},\tau)&=j_z(\tau)-\frac{1}{2}M\Omega_\parallel V_z(\boldsymbol{\xi},\tau),\end{aligned}\tag{C14}$$

and couples to the path $\mathbf{x}(\tau)$ only. With expression (C10) for the generating functional, and action (C13), we have derived a representation similar to Eq. (A1) with action (A2), extended by an additional oscillator in the z direction. We identify

$$j_x\equiv J_x,\quad j_y\equiv J_y.\tag{C15}$$

Inserting substitutions (C15) into solution (A8) for the generating functional in two dimensions, and performing the usual calculation for a harmonic oscillator with external source (Ref. [17] Chaps. 3 and 5) in the z direction, we obtain an intermediate result for the generating functional in three dimensions [Eq. (C2)]:

$$Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j},\mathbf{v}]=\lambda_{\mathrm{th}}^{-3}\,Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\int d^3\xi\exp\left\{\frac{M}{2\hbar}\int_0^{\hbar\beta}d\tau\,\mathbf{V}^2(\boldsymbol{\xi},\tau)\right\}\times\exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\;\mathbf{J}(\boldsymbol{\xi},\tau)\times\mathbf{G}^{\mathbf{x}_0}(\tau,\tau')\,\mathbf{J}(\boldsymbol{\xi},\tau')\right\}.\tag{C16}$$

The partition function follows from Eqs. (A17) and (A24),

$$Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=Z_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[0,0]=\frac{\hbar\beta\Omega_+/2}{\sinh\hbar\beta\Omega_+/2}\,\frac{\hbar\beta\Omega_-/2}{\sinh\hbar\beta\Omega_-/2}\,\frac{\hbar\beta\Omega_\parallel/2}{\sinh\hbar\beta\Omega_\parallel/2},\tag{C17}$$

and $\mathbf{G}^{\mathbf{x}_0}(\tau,\tau')$ is the 3×3 matrix of Green functions:

$$\mathbf{G}^{\mathbf{x}_0}(\tau,\tau')=\begin{pmatrix}G_{xx}^{\mathbf{x}_0}(\tau,\tau') & G_{xy}^{\mathbf{x}_0}(\tau,\tau') & 0\\ G_{yx}^{\mathbf{x}_0}(\tau,\tau') & G_{yy}^{\mathbf{x}_0}(\tau,\tau') & 0\\ 0 & 0 & G_{zz}^{\mathbf{x}_0}(\tau,\tau')\end{pmatrix}.\tag{C18}$$

Except for $G_{zz}^{\mathbf{x}_0}(\tau,\tau')$, the Green functions are given by the expressions in Eqs. (A22) and (A28). The Green function of the pure harmonic oscillator in the z direction,

$$G_{zz}^{\mathbf{x}_0}(\tau,\tau')=\frac{1}{M\beta\Omega_\parallel^2}\left(\frac{\hbar\beta\Omega_\parallel}{2}g_\parallel(\tau,\tau')-1\right),\tag{C19}$$

follows directly from limit (A23). Since the current $\mathbf{J}$ in Eq. (C14) still depends on time derivatives of $\mathbf{V}$, we have to perform some partial integrations in functional (C16). This is a very extensive but straightforward work, and thus we only present an instructive example. For that we apply the properties and the time derivatives of the Green functions which we presented in Appendix B. Consider the integral

$$I=-\frac{M^2}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\;\dot{V}_i(\boldsymbol{\xi},\tau)\,G_{ii}^{\mathbf{x}_0}(\tau,\tau')\,\dot{V}_i(\boldsymbol{\xi},\tau')\tag{C20}$$

occuring in the second exponential of Eq. (C16) with $i\in\{x,y,z\}$. A partial integration in the τ' integral leads to

$$\begin{aligned}I&=-\frac{M^2}{2\hbar^2}\int_0^{\hbar\beta}d\tau\,\dot{V}_i(\boldsymbol{\xi},\tau)\left(G_{ii}^{\mathbf{x}_0}(\tau,\tau')\,V_i(\boldsymbol{\xi},\tau')\Big|_{\tau'=0}^{\tau'=\hbar\beta}-\int_0^{\hbar\beta}d\tau'\frac{\partial G_{ii}^{\mathbf{x}_0}(\tau,\tau')}{\partial\tau'}V_i(\boldsymbol{\xi},\tau')\right)\\&=\frac{M^2}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,\dot{V}_i(\boldsymbol{\xi},\tau)\,G^{\cdot\mathbf{x}_0}_{ii}(\tau,\tau')\,V_i(\boldsymbol{\xi},\tau').\end{aligned}\tag{C21}$$

The surface term in the first line vanishes as a consequence of the periodicity of the current (C5) and Green function (B5). A second partial integration, now in the τ integral, results in

$$I=-\frac{M^2}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,V_i(\boldsymbol{\xi},\tau)\,\dot{G}^{\mathbf{x}_0}_{ii}(\tau,\tau')\,V_i(\boldsymbol{\xi},\tau')$$

$$=-\frac{M^2}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,V_i(\boldsymbol{\xi},\tau)\,\dot{\tilde{G}}^{\mathbf{x}_0}_{ii}(\tau,\tau')\,V_i(\boldsymbol{\xi},\tau')$$

$$-\frac{M}{2\hbar}\int_0^{\hbar}d\tau\,V_i^2(\boldsymbol{\xi},\tau). \tag{C22}$$

Here we have applied the periodicity property of the right-hand derivative of Green function (B19), leading to a vanishing surface term in this case too. In the second line, we have used the decomposition (B9) of the double-sided differentiated Green function. Note that the last term just cancels the appropriate term in the first exponential of the right-hand side of Eq. (C16). Eventually, after performing all such partial integrations, we reexpress Eq. (C16) by

$$Z_{\boldsymbol{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j},\mathbf{v}]=\lambda_{\mathrm{th}}^{-3}\,Z_{\boldsymbol{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\int d^3\xi\exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\right.$$

$$\left.\times\tilde{\mathbf{s}}(\boldsymbol{\xi},\tau)\,\mathbf{H}^{\mathbf{x}_0}(\tau,\tau')\,\tilde{\mathbf{s}}(\boldsymbol{\xi},\tau')\right\}, \tag{C23}$$

with six-dimensional sources

$$\tilde{\mathbf{s}}(\boldsymbol{\xi},\tau)=(\mathbf{j}(\tau),\mathbf{V}(\boldsymbol{\xi},\tau)) \tag{C24}$$

and the 6×6 matrix $\mathbf{H}^{\mathbf{x}_0}(\tau,\tau')$, which has no significance as long as we have not done the $\boldsymbol{\xi}$ integration. We explicitly insert decomposition (C8) into expression (C24) of the source vector $\tilde{\mathbf{s}}$. Since $\mathbf{v}_0(\boldsymbol{\xi})$ from Eq. (C7) is constant in time, some temporal integrals in the exponential of Eq. (C23) can be calculated, and we obtain

$$Z_{\boldsymbol{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j},\mathbf{v}]=\lambda_{\mathrm{th}}^{-3}\,Z_{\boldsymbol{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,\mathbf{s}(\tau)\right.$$

$$\left.\times\mathbf{H}^{\mathbf{x}_0}(\tau,\tau')\,\mathbf{s}(\tau')\right\}\int d^3\xi$$

$$\times\exp\left\{-\frac{M}{2\hbar^2\beta}\boldsymbol{\xi}^2+i\frac{M}{\hbar^2\beta}\boldsymbol{\xi}\cdot\int_0^{\hbar\beta}d\tau\,\mathbf{v}(\tau)\right\} \tag{C25}$$

with the new six vector

$$\mathbf{s}(\tau)=(\mathbf{j}(\tau),\mathbf{v}(\tau)) \tag{C26}$$

consisting of the original sources $\mathbf{j}$ and $\mathbf{v}$ only. The Gaussian ξ integral in Eq. (C25) can be easily solved, and the terms appearing from quadratic completion modify the above matrix $\mathbf{H}^{\mathbf{x}_0}(\tau,\tau')$. The final result for the generating functional of all position and momentum dependent correlations is given by

$$Z_{\boldsymbol{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}[\mathbf{j},\mathbf{v}]=Z_{\boldsymbol{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\exp\left\{\frac{1}{2\hbar^2}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\right.$$

$$\left.\times\mathbf{s}(\tau)\,\mathbf{G}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')\,\mathbf{s}(\tau')\right\}. \tag{C27}$$

The complete 6×6 matrix $\mathbf{G}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')$ contains all possible Green functions describing position-position, position-momentum, and momentum-momentum correlations. As a consequence of separating the fluctuations into those perpendicular and parallel to the direction of the magnetic field, all correlations between x and y on the one hand and z on the other hand vanish, as well as those for the appropriate momenta. The symmetries for the position-position Green functions and their derivatives were investigated in detail in Appendix B, and lead to a further reduction of the number of significant matrix elements. It turns out that only nine elements are independent of each other. Therefore we can write the matrix

$$\mathbf{G}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')=\begin{pmatrix}
G_{xx}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & G_{xy}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & 0 & G_{xp_x}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & G_{xp_y}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & 0\\
G_{xy}^{\mathbf{p}_0,\mathbf{x}_0}(\tau',\tau) & G_{xx}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & 0 & -G_{xp_y}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & G_{xp_x}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & 0\\
0 & 0 & G_{zz}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & 0 & 0 & G_{zp_z}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')\\
G_{xp_x}^{\mathbf{p}_0,\mathbf{x}_0}(\tau',\tau) & -G_{xp_y}^{\mathbf{p}_0,\mathbf{x}_0}(\tau',\tau) & 0 & G_{p_xp_x}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & G_{p_xp_y}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & 0\\
G_{xp_y}^{\mathbf{p}_0,\mathbf{x}_0}(\tau',\tau) & G_{xp_x}^{\mathbf{p}_0,\mathbf{x}_0}(\tau',\tau) & 0 & G_{p_xp_y}^{\mathbf{p}_0,\mathbf{x}_0}(\tau',\tau) & G_{p_xp_x}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau') & 0\\
0 & 0 & G_{zp_z}^{\mathbf{p}_0,\mathbf{x}_0}(\tau',\tau) & 0 & 0 & G_{p_zp_z}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')
\end{pmatrix}. \tag{C28}$$

The matrix decays into four 3×3 blocks, each of which describes another type of correlation: the upper left a position-position correlation, the upper right (as well as the lower left) position-momentum correlation, and the lower right a momentum-momentum correlation. The different elements of the matrix are

$$G_{xx}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')=\langle\tilde{x}(\tau)\tilde{x}(\tau')\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=G_{xx}^{\mathbf{x}_0}(\tau,\tau'), \quad \text{(C29)}$$

$$G_{xy}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')=\langle\tilde{x}(\tau)\tilde{y}(\tau')\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=G_{xy}^{\mathbf{x}_0}(\tau,\tau'), \quad \text{(C30)}$$

$$G_{zz}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')=\langle\tilde{z}(\tau)\tilde{z}(\tau')\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=G_{zz}^{\mathbf{x}_0}(\tau,\tau'), \quad \text{(C31)}$$

$$\begin{aligned}G_{xp_x}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')&=\langle\tilde{x}(\tau)\tilde{p}_x(\tau')\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\\&=iMG_{xx}^{\bullet\mathbf{x}_0}(\tau,\tau')-M\Omega_B G_{xy}^{\mathbf{x}_0}(\tau,\tau')\\&=\frac{\hbar}{4i}\{\Theta(\tau-\tau')[h_+(\tau,\tau')+h_-(\tau,\tau')]\\&\quad-\Theta(\tau'-\tau)[h_+(\tau',\tau)+h_-(\tau',\tau)]\},\end{aligned} \quad \text{(C32)}$$

$$\begin{aligned}G_{xp_y}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')&=\langle\tilde{x}(\tau)\tilde{p}_y(\tau')\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\\&=iMG_{xy}^{\bullet\mathbf{x}_0}(\tau,\tau')+M\Omega_B G_{xx}^{\mathbf{x}_0}(\tau,\tau')\\&=-\frac{\hbar}{4}[g_+(\tau,\tau')-g_-(\tau,\tau')]-\frac{1}{\beta}\frac{\Omega_B}{\Omega_+\Omega_-},\end{aligned} \quad \text{(C33)}$$

$$\begin{aligned}G_{zp_z}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')&=\langle\tilde{z}(\tau)\tilde{p}_z(\tau')\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=iMG_{zz}^{\bullet\mathbf{x}_0}(\tau,\tau')\\&=\frac{\hbar}{2i}[\Theta(\tau-\tau')h_\parallel(\tau,\tau')-\Theta(\tau'-\tau)h_\parallel(\tau',\tau)],\end{aligned} \quad \text{(C34)}$$

$$\begin{aligned}G_{p_xp_x}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')&=\langle\tilde{p}_x(\tau)\tilde{p}_x(\tau')\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}\\&=-M^{2\bullet}\tilde{G}_{xx}^{\bullet\mathbf{x}_0}(\tau,\tau')-2iM^2\Omega_B{}^{\bullet}G_{xy}^{\mathbf{x}_0}(\tau,\tau')\\&\quad+M^2\Omega_B^2G_{xx}^{\mathbf{x}_0}(\tau,\tau')-\frac{M}{\beta}\\&=\frac{\hbar M\Omega_\perp}{4}[g_+(\tau,\tau')+g_-(\tau,\tau')]\\&\quad-\frac{M}{\beta}\left(1-\frac{\Omega_B^2}{\Omega_+\Omega_-}\right),\end{aligned} \quad \text{(C35)}$$

$$\begin{aligned}G_{p_xp_y}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')&=\langle\tilde{p}_x(\tau)\tilde{p}_y(\tau')\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=2iM^2\Omega_B{}^{\bullet}G_{xx}^{\mathbf{x}_0}(\tau,\tau')\\&\quad-M^{2\bullet}G_{xy}^{\bullet\mathbf{x}_0}(\tau,\tau')+M^2\Omega_B^2G_{xy}^{\mathbf{x}_0}(\tau,\tau')\\&=\frac{\hbar M\Omega_\perp}{4i}\{\Theta(\tau-\tau')[h_+(\tau,\tau')-h_-(\tau,\tau')]\\&\quad-\Theta(\tau'-\tau)[h_+(\tau',\tau)-h_-(\tau',\tau)]\},\end{aligned} \quad \text{(C36)}$$

$$\begin{aligned}G_{p_zp_z}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')&=\langle\tilde{p}_z(\tau)\tilde{p}_z(\tau')\rangle_{\mathbf{\Omega}}^{\mathbf{p}_0,\mathbf{x}_0}=-M^{2\bullet}\tilde{G}_{zz}^{\bullet\mathbf{x}_0}(\tau,\tau')-\frac{M}{\beta}\\&=\frac{\hbar M\Omega_\parallel}{2}g_\parallel(\tau,\tau')-\frac{M}{\beta},\end{aligned} \quad \text{(C37)}$$

where the expectation values are defined by Eq. (3.12). Note that all these Green functions are invariant under time translations, such that

$$G_{\mu\nu}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')=G_{\mu\nu}^{\mathbf{p}_0,\mathbf{x}_0}(\tau-\tau') \quad \text{(C38)}$$

with $\mu,\nu\in\{x,y,z,p_x,p_y,p_z\}$.

It is quite instructive to prove that all these Green functions can be decomposed into quantum-statistical and classical parts as we did it in Eq. (A22). Since we know that the classical correlation functions do not depend on the Euclidean time, all derivative terms in Eqs. (C29)–(C37) do not contribute a classical term. We can write each Green function as

$$G_{\mu\nu}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')=G_{\mu\nu}^{\mathrm{qm}}(\tau,\tau')-G_{\mu\nu}^{\mathrm{cl}}. \quad \text{(C39)}$$

This relation was already checked for Eqs. (C29)–(C31) in Appendix A. The classical contribution is zero in Eqs. (C32), (C34), and (C36) following from the absence of classical terms in derivatives of the Green functions and mixed correlations like Eq. (A30). It seems surprising that correlation (C33) contains a classical term, while Eq. (C32) possesses none. This is, however, a consequence of the cross product of the orbital angular momentum appearing in action (C3), and the explicit classical calculation entails

$$G_{xp_x}^{\mathrm{cl}}=\langle xp_x\rangle^{\mathrm{cl}}=0, \quad G_{xp_y}^{\mathrm{cl}}=\langle xp_y\rangle^{\mathrm{cl}}=\frac{1}{\beta}\frac{\Omega_B}{\Omega_\perp^2-\Omega_B^2}, \quad \text{(C40)}$$

where the latter is the subtracted classical term in Eq. (A22) when considering the first two substitutions in Eq. (C15). In Eq. (C37), the second term is obviously the classical one, since

$$G_{p_zp_z}^{\mathrm{cl}}=\langle p_zp_z\rangle^{\mathrm{cl}}=\frac{M}{\beta}. \quad \text{(C41)}$$

The extraction of the classical terms

$$G_{p_xp_x}^{\mathrm{cl}}=\langle p_xp_x\rangle^{\mathrm{cl}}=\frac{M}{\beta}\left(1+\frac{\Omega_B^2}{\Omega_\perp^2-\Omega_B^2}\right) \quad \text{(C42)}$$

in the case of the Green function $G_{p_xp_x}^{\mathbf{p}_0,\mathbf{x}_0}(\tau,\tau')$ requires the consideration of the last two terms in Eq. (C35). Thus we have shown that the decomposition (C39) holds for each of the Green functions (C29)–(C37). Note the necessity of subtracting the classical terms since they all diverge in the classical limit of high temperatures ($\beta\to0$).

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