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Rotating highly mixed Gaussian packets with minimal energy

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We study two-dimensional quantum mixed Gaussian packets with a fixed value of mean angular momentum. Highly mixed packets, minimizing the mean energy of an isotropic oscillator with fixed mean angular momentum $\mathcal{L}$, are found under the condition that the inverse purity $\mathcal{P}^{-1}$ exceeds the sum $1+2\mathcal{L}$. These states can be considered rotating thermal states. Their statistical properties (such as variances of angular momentum and energy) are studied. The case of a charged particle in a homogeneous magnetic field is considered as well.

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I. INTRODUCTION

Studies of quantum Gaussian wave packets are as old as quantum mechanics itself [1–3]. In particular, many properties of multidimensional packets have been discussed in detail, e.g., in original papers, books, and reviews [4–12]. More recently, the interest in such packets has been revived in connection with the problems posed by quantum information (in particular, entanglement and separability) [13–27]. Rotating Gaussian packets or Gaussian packets in rotating frames were studied in [28–33]. Other packets describing massive quantum particles with nonzero orbital angular momentum ("vortex states") were considered in [33–39]. Recently such states were created in different experiments with electrons [40–44] and neutrons [45]. It is pointed out in the cited papers that matter wave beams with orbital angular momentum can find applications in areas such as condensed-matter spectroscopy, electron microscopy, and particle physics. In particular, they can be used in the study of magnetic properties of materials and for the manipulation of nanoparticles.

Searches for quantum states minimizing some physical quantities or possessing certain distinguished properties gave rise to the discovery of several useful new concepts. For example, the Gaussian nonspreading packets of the harmonic oscillator introduced by Schrödinger [1] (they minimize the Heisenberg-Weyl uncertainty relation) resulted, after many years, in the concept of coherent states [46]. The search for more general *minimum uncertainty states* [47,48], realizing the equality in the Heisenberg-Weyl uncertainty relation, resulted in the important concept of squeezed states [49], although such states were considered for the first time by Kennard [2] and later by Husimi [50] and Plebański [51]. Nonspreading packets of a charged particle in a uniform magnetic field, considered by Darwin [3] and Husimi [50], were generalized later as coherent states in a magnetic field [52–54]. The nonzero mean value of the angular momentum operator is the distinguishing feature of these states.

The problem of finding quantum states that minimize uncertainty products under additional constraints was raised in [55], where the constraint was the correlation coefficient between the coordinate and the momentum operators. The corresponding correlated quantum states play an important role in the problems of quantum measurements [56–58], quantum tunneling [59], and low-energy nuclear reactions [60]. Minimization of the uncertainty product for *mixed quantum states* of a fixed *purity* was considered in [12] and [61–68].

The subject of this paper is an intersection among the directions mentioned above. The aim is to find two-dimensional Gaussian packets possessing the minimal possible mean energy under the constraint of a fixed value of mean angular momentum. This problem was solved in [69] for pure quantum states. Here we consider mixed quantum states. Although we have not yet succeeded in finding the complete solution to the problem, we have obtained a nice analytical solution for highly mixed packets (the definition is given in the text). Such packets can be interpreted as *rotating thermal states*, and we believe that they are of interest to many readers.

The plan of the paper is as follows. Section II is devoted to general properties of two-dimensional mixed Gaussian packets in the coordinate and Wigner representations. The main problem of energy minimization under the constraint of the fixed mean angular momentum is considered in Sec. III. It is known that the Wigner function formalism is the most suitable one for treating many problems related to properties of Gaussian states. It is curious, however, that the formalism of density matrices in the coordinate representation turns out to be more adequate for solving the specific problem under study. This is because the Wigner function is "too symmetrical" with respect to the coordinate and momentum variables, so that it is difficult to find a simple way of solving many coupled minimization equations in the Wigner representation. On the contrary, the equations in the coordinate representation can be solved step by step. We find an analytical exact solution for highly mixed states, which are reduced to thermal states in the case of zero mean angular momentum. The statistical properties of these states are studied in Sec. IV. Section V is devoted to the minimal energy Gaussian packets for a charged oscillator and a charged free particle in a homogeneous magnetic field. The last section (VI) is devoted to the discussion of the results obtained and directions of possible future studies. Details of some cumbersome calculations and explicit expressions for variances are given in Appendixes A and B.

II. TWO-DIMENSIONAL HOMOGENEOUS GAUSSIAN MIXED STATES

Let us consider two-dimensional mixed Gaussian states with zero mean values of coordinates and momenta. They

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are described by means of the density matrix [matrix elements $\rho(\mathbf{r},\mathbf{r}') \equiv \langle \mathbf{r}|\hat\rho|\mathbf{r}'\rangle$ of the Hermitian statistical operator $\hat\rho$ in the coordinate representation]

$$\rho(\mathbf{r},\mathbf{r}') = \tilde N \exp\left[-\tfrac{1}{2}(\mathbf{r}A\mathbf{r} + 2\mathbf{r}B\mathbf{r}' + \mathbf{r}'A^*\mathbf{r}')\right]. \qquad (1)$$

Here $\mathbf{r} = (x,y)$ and $\mathbf{r}' = (x',y')$. It is convenient to use dimensionless variables in order to simplify formulas. Having in mind applications to the quantum isotropic harmonic oscillator with mass M and frequency ω, the symbols x and y hereafter mean normalized coordinates obtained from the dimensional variables x_d and y_d by means of the scaling transformation $x = x_d(M\omega/\hbar)^{1/2}$ and $y = y_d(M\omega/\hbar)^{1/2}$, where $\hbar$ is the Planck constant. This scaling transformation implies that hereafter formally $\hbar = 1$. Therefore the 2×2 matrices A and B are dimensionless. Complex matrix A is symmetrical, whereas the Hermiticity of the density matrix, $\rho(\mathbf{r},\mathbf{r}') = \rho^*(\mathbf{r}',\mathbf{r})$ (the asterisk indicates complex conjugation), imposes the restriction of Hermiticity on matrix $B = B^\dagger$. The probability density equals

$$\rho(\mathbf{r},\mathbf{r}) = \tilde N \exp[-\mathbf{r}\mathrm{Re}(A+B)\mathbf{r}] \qquad (2)$$

[obviously matrix $\mathrm{Re}(B)$ is symmetrical]. Consequently, the normalization condition $\mathrm{Tr}(\hat\rho) = \int dxdy\rho(\mathbf{r},\mathbf{r}) = 1$ implies the value

$$\tilde N = \sqrt{\det \mathrm{Re}(A+B)}/\pi \equiv \sqrt{\Delta}/\pi. \qquad (3)$$

It is convenient to separate the real and imaginary parts of matrices A and B as follows:

$$A = \left\| \begin{matrix} a_{11} + i\chi_{11} & a_{12} + i\chi_{12} \\ a_{12} + i\chi_{12} & a_{22} + i\chi_{22} \end{matrix} \right\|, \qquad (4)$$

$$B = \left\| \begin{matrix} b_{11} & b_{12} + i\gamma \\ b_{12} - i\gamma & b_{22} \end{matrix} \right\|. \qquad (5)$$

Then

$$\Delta = \alpha_{11}^{+}\alpha_{22}^{+} - (\alpha_{12}^{+})^2, \quad \alpha_{jk}^{\pm} \equiv a_{jk} \pm b_{jk}. \qquad (6)$$

The purity $\mathcal{P} = \mathrm{Tr}(\hat\rho^2)$ can be calculated as

$$\mathcal{P} = \int dxdydx'dy'\rho(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}',\mathbf{r})$$
$$= \tilde N^2 \int dxdydx'dy' \exp(-\mathbf{R}G\mathbf{R}) = \frac{\Delta}{\sqrt{\det(G)}}, \qquad (7)$$

where $\mathbf{R} = (\mathbf{r},\mathbf{r}')$ and the 4×4 matrix G has the following block form:

$$G = \left\| \begin{matrix} \mathrm{Re}(A) & \mathrm{Re}(B) \\ \mathrm{Re}(B) & \mathrm{Re}(A) \end{matrix} \right\|. \qquad (8)$$

The determinant of the block matrix having this structure can be written as

$$\det(G) = \det[\mathrm{Re}(A+B)]\det[\mathrm{Re}(A-B)].$$

Therefore

$$\mathcal{P} = \sqrt{\frac{\det[\mathrm{Re}(A+B)]}{\det[\mathrm{Re}(A-B)]}} = \sqrt{\frac{\alpha_{11}^{+}\alpha_{22}^{+} - (\alpha_{12}^{+})^2}{\alpha_{11}^{-}\alpha_{22}^{-} - (\alpha_{12}^{-})^2}}. \qquad (9)$$

Let us introduce the notation $\overline{uv} \equiv \langle \hat u\hat v + \hat v\hat u\rangle/2 - \langle\hat u\rangle\langle\hat v\rangle$ for the symmetrical covariances of the arbitrary Hermitian operators $\hat u$ and $\hat v$ [where $\langle\hat u\rangle \equiv \mathrm{Tr}(\hat\rho\hat u)$]. Then we can construct the 4×4 symmetrical covariance matrix of coordinates and momentum operators

$$\mathcal{M} = \left\| \begin{matrix} \mathcal{M}_p & \mathcal{M}_{pq} \\ \mathcal{M}_{qp} & \mathcal{M}_q \end{matrix} \right\|, \qquad (10)$$

consisting of the 2×2 blocks

$$\mathcal{M}_p = \left\| \begin{matrix} \overline{p_x^2} & \overline{p_xp_y} \\ \overline{p_xp_y} & \overline{p_y^2} \end{matrix} \right\|, \quad \mathcal{M}_q = \left\| \begin{matrix} \overline{x^2} & \overline{xy} \\ \overline{xy} & \overline{y^2} \end{matrix} \right\|,$$

$$\mathcal{M}_{pq} = \left\| \begin{matrix} \overline{p_xx} & \overline{p_xy} \\ \overline{xp_y} & \overline{p_yy} \end{matrix} \right\| = \mathcal{M}_{qp}^T,$$

where $\mathcal{M}^T$ indicates the transposed matrix. The elements in the matrices introduced above can be calculated either directly from the density matrix, (1), or by comparing Eq. (1) with the equivalent form given in [12],

$$\rho(\mathbf{r}_2,\mathbf{r}_1) = (2\pi)^{-1}(\det\mathcal{M}_q)^{-1/2}\exp\left[i\delta\mathbf{r}\mathcal{M}_{pq}\mathcal{M}_q^{-1}\mathbf{r}\right.$$
$$\left. - \tfrac{1}{2}\delta\mathbf{r}\left(\mathcal{M}_p - \mathcal{M}_{pq}\mathcal{M}_q^{-1}\mathcal{M}_{qp}\right)\delta\mathbf{r} - \tfrac{1}{2}\mathbf{r}\mathcal{M}_q^{-1}\mathbf{r}\right], \qquad (11)$$

where $\mathbf{r} = (\mathbf{r}_2 + \mathbf{r}_1)/2$ and $\delta\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$. The explicit expressions are given in Appendix A.

The covariance matrix $\mathcal{M}$ completely determines the Gaussian Wigner function [8,9,12,70]:

$$W(\mathbf{q}) = (\det\mathcal{M})^{-1/2}\exp\left[-\tfrac{1}{2}(\mathbf{q} - \langle\mathbf{q}\rangle)\mathcal{M}^{-1}(\mathbf{q} - \langle\mathbf{q}\rangle)\right]. \qquad (12)$$

Here $\mathbf{q} \equiv (\mathbf{p},\mathbf{r})$ (we put $\langle\mathbf{q}\rangle = 0$ in this section). We use the following definition:

$$W(\mathbf{r},\mathbf{p}) = \int d\mathbf{v}\rho(\mathbf{r} + \mathbf{v}/2, \mathbf{r} - \mathbf{v}/2)\exp(-i\mathbf{p}\mathbf{v}),$$
$$\int W(\mathbf{r},\mathbf{p})d\mathbf{r}d\mathbf{p}/(2\pi)^2 = 1.$$

The purity of Gaussian states is also determined completely by the covariance matrix [9,12]:

$$\mathcal{P} = \int W^2(\mathbf{r},\mathbf{p})\frac{d\mathbf{r}d\mathbf{p}}{(2\pi)^2} = \frac{1}{4}(\det\mathcal{M})^{-1/2}. \qquad (13)$$

The requirement that $\mathcal{P} \leqslant 1$ imposes, in view of Eq. (9), the following restriction on the real elements of "mixing matrix" B:

$$b_{11}a_{22} + b_{22}a_{11} - 2b_{12}a_{12} \leqslant 0. \qquad (14)$$

According to Eq. (9), the purity does not depend on the parameters γ and χ_{jk}, i.e., the imaginary parts of matrices B and A. However, these parameters cannot be chosen at will, because the statistical operator $\hat\rho$ must be *nonnegatively definite*. The consequence of this property is the nonnegative definiteness of matrix $\mathcal{M} - i\Sigma/2$ [9,12,13,19,71,72], where the antisymmetric matrix Σ (determined by the commutators of coordinates and momentum operators) has the following block form:

$$\Sigma = \left\| \begin{matrix} 0 & I_2 \\ -I_2 & 0 \end{matrix} \right\|, \quad I_2 = \left\| \begin{matrix} 1 & 0 \\ 0 & 1 \end{matrix} \right\|. \qquad (15)$$

One of the consequences of this nonnegativity is the inequality

$$\mathcal{D}_0 \equiv \det\mathcal{M} \geqslant 1/16, \qquad (16)$$

which is equivalent to $\mathcal{P} \leqslant 1$. Other consequences are the Schrödinger-Robertson uncertainty relations

$$U_x \equiv \overline{x^2}\,\overline{p_x^2} - (\overline{xp_x})^2 \geqslant 1/4, \quad U_y \geqslant 1/4. \tag{17}$$

The explicit forms of U_x and U_y are

$$U_x = \frac{1}{4\Delta}(\alpha_{11}^-\alpha_{22}^+ + \chi_+^2), \quad U_y = \frac{1}{4\Delta}(\alpha_{22}^-\alpha_{11}^+ + \chi_-^2),$$

where $\chi_\pm = \chi_{12} \pm \gamma$.

In the case of two spatial dimensions, there exists one more important inequality [12]:

$$\mathcal{D}_0 - \mathcal{D}_2/4 + 1/16 \geqslant 0, \tag{18}$$

with

$$\mathcal{D}_2 \equiv U_x + U_y + 2\overline{xy}\,\overline{p_xp_y} - 2\,\overline{xp_y}\,\overline{yp_x}. \tag{19}$$

We have explicitly

$$\mathcal{D}_2 = \frac{1}{4\Delta}(\alpha_{11}^-\alpha_{22}^+ + \alpha_{22}^-\alpha_{11}^+ - 2\alpha_{12}^-\alpha_{12}^+ + 4\gamma^2), \tag{20}$$

so that relation (18) together with (9) and (20) results in a remarkable inequality, containing elements of mixing matrix B only:

$$b_{11}b_{22} - b_{12}^2 - \gamma^2 \geqslant 0. \tag{21}$$

III. MINIMAL ENERGY HOMOGENEOUS PACKETS WITH A FIXED MEAN ANGULAR MOMENTUM

The dimensionless Hamiltonian of the isotropic harmonic oscillator reads

$$\hat{H} = \frac{1}{2}\big(\hat{p}_x^2 + \hat{p}_y^2 + \hat{x}^2 + \hat{y}^2\big). \tag{22}$$

Using explicit expressions, given in Appendix A, the mean energy in state (1) can be written as

$$\mathcal{E} = \frac{1}{4\Delta}[\alpha_{11}^+ + \alpha_{22}^+ + (\alpha_{11}^- + \alpha_{22}^-)\Delta + f(\chi_{jk})], \tag{23}$$

where

$$f(\chi_{jk}) = \alpha_{11}^+\big(\chi_{22}^2 + \chi_+^2\big) + \alpha_{22}^+\big(\chi_{11}^2 + \chi_-^2\big) - 2\alpha_{12}^+(\chi_{11}\chi_+ + \chi_{22}\chi_-). \tag{24}$$

Our goal is to minimize function (23) for the fixed mean value of the angular momentum operator $\mathcal{L} = \langle \hat{x}\hat{p}_y - \hat{y}\hat{p}_x\rangle$, which can be written as

$$\mathcal{L} = [\alpha_{12}^+(\chi_{22} - \chi_{11}) + \alpha_{11}^+\chi_+ - \alpha_{22}^+\chi_-]/(2\Delta). \tag{25}$$

The minimization procedure, described in detail in Appendix B, results in the formula

$$2\mathcal{E} = \frac{g^3}{\Delta^2} - g\mathcal{L}^2 + 2\gamma\mathcal{L} + \sqrt{g^2 + 4\kappa\Delta} - \frac{2\kappa\eta^2}{\sqrt{g^2 + 4\kappa\Delta}}, \tag{26}$$

where nonnegative parameters g and η^2 satisfy the equations

$$\gamma^2 = \mathcal{L}^2\Delta - \frac{\eta^2}{\Delta} + \frac{\eta^2}{g}\sqrt{g^2 + 4\kappa\Delta}, \tag{27}$$

$$g(\mathcal{L}g - \gamma)^2 = \eta^4\left(\frac{g}{\Delta^2} - \frac{2\kappa}{\sqrt{g^2 + 4\kappa\Delta}}\right), \tag{28}$$

with

$$\Delta \equiv g^2 - \eta^2 > 0, \quad \kappa \equiv (\mathcal{P}^{-2} - 1)/4 \geqslant 0. \tag{29}$$

Solving Eqs. (27) and (28) with respect to variables g and η, for arbitrary values of parameters γ, $\mathcal{L}$, and κ, one could obtain the function $\mathcal{E}(\gamma,\mathcal{L},\kappa)$ and minimize it with respect to γ under the additional restriction

$$|\gamma| \leqslant \frac{2\kappa\Delta}{g + \sqrt{g^2 + 4\kappa\Delta}}, \tag{30}$$

which is the consequence of inequality (21) and Eq. (B9). Unfortunately, Eqs. (27) and (28) are too complicated to be solved analytically in the most general case. Therefore we analyze below some special cases, admitting exact or approximate solutions.

A. Pure quantum states

The first case corresponds to pure quantum states with $\kappa = \gamma = b_{jk} = 0$. Then Eq. (28) yields $\eta^2 = g|\mathcal{L}|\Delta$, so that $\eta^2 = g^3|\mathcal{L}|/(1 + g|\mathcal{L}|)$ and $\Delta = g^2/(1 + g|\mathcal{L}|)$. Putting these expressions in (27), we arrive at the equation $g|\mathcal{L}|(g^2 - 1) = 0$. Consequently,

$$g = 1, \quad \eta^2 = |\mathcal{L}|/(1 + |\mathcal{L}|). \tag{31}$$

Then Eq. (26) yields

$$\mathcal{E}_{\text{min}}^{\text{pure}} = 1 + |\mathcal{L}|. \tag{32}$$

This result was obtained in [69], where the properties of the corresponding mimimal energy pure packets were studied in detail.

B. Highly mixed rotating thermal packets

One can also note that Eqs. (27) and (28) are satisfied for any value of parameter κ, if one puts $\eta = 0$ and $\gamma = g\mathcal{L}$. Then Eq. (26) takes the form

$$2\mathcal{E} = \frac{1}{g} + g(\mathcal{L}^2 + \sqrt{1 + 4\kappa}) = \frac{1}{g} + g(\mathcal{L}^2 + \mathcal{P}^{-1}). \tag{33}$$

The right-hand side of (33) attains the minimum for

$$g = g_* \equiv \sqrt{\mathcal{P}/(1 + \mathcal{P}\mathcal{L}^2)}. \tag{34}$$

Therefore

$$\mathcal{E}_{\text{min}}^{\text{mix}} = g_*^{-1} = \sqrt{\mathcal{L}^2 + \mathcal{P}^{-1}} = \sqrt{(1 + \mathcal{L}^2\mathcal{P})/\mathcal{P}}. \tag{35}$$

If $\mathcal{L} = 0$, (35) coincides with the mean energy of the two-dimensional isotropic oscillator in the equilibrium (thermal) state, possessing purity $\mathcal{P}$. Consequently, the minimal energy state with zero mean angular momentum and fixed purity is the thermal state. Therefore it seems natural to call the states obtained *rotating thermal states*.

Note, however, that (35) does not go to (32) if $\mathcal{P} = 1$ but $\mathcal{L} \neq 0$. The reason is that the equality $\gamma = g\mathcal{L}$ is consistent (for $\eta = 0$) with (21) and (30) under the restrictions

$$\mathcal{P}^{-1} \geqslant 1 + 2|\mathcal{L}|, \quad \kappa \geqslant |\mathcal{L}|(|\mathcal{L}| + 1). \tag{36}$$

Consequently, the simple formula (35) is valid for highly mixed states satisfying (36). Then $\sqrt{\mathcal{L}^2 + \mathcal{P}^{-1}} \geqslant 1 + |\mathcal{L}|$. If

$\mathcal{L}=0$, then

$$\mathcal{E}_{\min}^{\rm mix}=\mathcal{P}^{-1/2}=(1+4\kappa)^{1/4}=1+\kappa-3\kappa^2/2+\dots. \tag{37}$$

C. Approximate lower bounds for weakly mixed states

If condition (36) is not satisfied, one can look for an approximate lower bound in the case of *weakly mixed states* with $\kappa \ll 1$. For this purpose, it is convenient to introduce new variables and parameters:

$$y=\eta^2/g^2\geqslant 0,\quad \Gamma=\gamma/g,\quad \mu=\mathcal{L}-\Gamma. \tag{38}$$

Then Eqs. (26)–(28) can be written as follows:

$$2\mathcal{E}/g=\frac{1}{g^2(1-y)}+\mathcal{L}^2(1-y)+(1+y)\sqrt{1+4\kappa(1-y)}-\frac{2\kappa y(1-y)}{\sqrt{1+4\kappa(1-y)}}, \tag{39}$$

$$\mu(2\mathcal{L}-\mu)=y\left[\mathcal{L}^2+\frac{1}{g^2(1-y)}-\sqrt{1+4\kappa(1-y)}\right], \tag{40}$$

$$\mu^2=y^2\left[\frac{1}{g^2(1-y)^2}-\frac{2\kappa}{\sqrt{1+4\kappa(1-y)}}\right]. \tag{41}$$

Rewriting Eq. (41) as

$$g^{-2}=(1-y)^2\left[\frac{\mu^2}{y^2}+\frac{2\kappa}{\sqrt{1+4\kappa(1-y)}}\right], \tag{42}$$

we put this value into Eq. (40), arriving at the equation

$$(\mu-\mathcal{L}y)^2=y^2\frac{1+2\kappa(1-y)}{\sqrt{1+4\kappa(1-y)}}. \tag{43}$$

We suppose here that $y\neq 0$ and $\mu\neq 0$ (otherwise we have the case considered in Sec. III B). The mean energy can now be written as

$$\mathcal{E}=\left[\frac{y}{1-y}\sqrt{1+4\kappa(1-y)}+\mathcal{L}\mu\right]\times\left[\mu^2+\frac{2\kappa y^2}{\sqrt{1+4\kappa(1-y)}}\right]^{-1/2}. \tag{44}$$

Equation (43) can be transformed into an algebraic equation of the sixth order with respect to variable y. It is hardly possible to find its analytical solutions for arbitrary parameters μ, $\mathcal{L}$, and κ. Therefore we look here for an approximate solution for weakly mixed states with $\kappa \ll 1$ (so that $|\Gamma|\ll 1$ as well). Let us assume for definiteness that $\mathcal{L}>0$. In this case, taking into account the results in Sec. III A, it seems reasonable to write $y=\mu f$ with $f=f_0+f_1+f_2+\dots$, where $f_0=(1+\mathcal{L})^{-1}$ and $f_j\sim O(\kappa^j)$ for $j=1,2,\dots$. Limiting ourselves to terms of the order of κ^2, we find

$$f_1=0,\quad f_2=-\frac{\kappa^2}{(1+2\mathcal{L})(1+\mathcal{L})^3}. \tag{45}$$

Putting these expressions into (44) and remembering that $\mu=\mathcal{L}-\Gamma$ (with $|\Gamma|\sim\kappa$), one can obtain, with the same accuracy, the function

$$\mathcal{E}(\kappa,\Gamma)=1+\mathcal{L}+\frac{\kappa}{1+\mathcal{L}}-\Gamma+\Gamma^2+\frac{\kappa\Gamma}{(1+\mathcal{L})^2}-\frac{\kappa^2(3+6\mathcal{L}+2\mathcal{L}^2)}{2(1+\mathcal{L})^3(2\mathcal{L}+1)}. \tag{46}$$

Here Γ is still a free parameter. Since $d\mathcal{E}/d\Gamma<0$ for small values of κ and Γ, the minimal value of the mean energy corresponds to the maximal permitted value of Γ. Inequality (30) in the case involved can be written as

$$\Gamma\leqslant\frac{2\kappa(1-y)}{1+\sqrt{1+4\kappa(1-y)}}\approx\kappa f_0(1+\Gamma-\kappa f_0). \tag{47}$$

Therefore $\Gamma\leqslant\kappa f_0$ within the accuracy of the approximation. Using this maximal value of Γ we find

$$\mathcal{E}_{\min}^{\rm mix}=1+\mathcal{L}+\frac{\kappa^2(1+4\mathcal{L}+2\mathcal{L}^2)}{2(1+\mathcal{L})^3(2\mathcal{L}+1)}. \tag{48}$$

This formula shows the influence of a small quantum mixing parameter $\kappa\ll 1$ on the minimal energy of Gaussian packets, provided $\mathcal{L}$ is not too small. In particular, $(\mathcal{E}_{\min}^{\rm mix}-\mathcal{E}_{\min}^{\rm pure})/\mathcal{E}_{\min}^{\rm pure}\approx\kappa^2/(2\mathcal{L}^3)$ if $\mathcal{L}\gg 1$.

One can note, however, that Eq. (48) does not go to (37) in the limit of $\mathcal{L}=0$. To understand this discrepancy, one should remember that variable y must be nonnegative, due to its definition. Therefore the solution in the form $y=\mu f$ with $f_0>0$ can be used under the restriction $\mu=\mathcal{L}-\Gamma>0$ only. Consequently, Eq. (48) is valid under the restriction $\kappa<\mathcal{L}$ (weakly mixed states). If $\mathcal{L}<\kappa\ll 1$, then the maximal value $\Gamma=\mathcal{L}$ transforms Eq. (46) to

$$\mathcal{E}_{\min}=1+\kappa-3\kappa^2/2+\mathcal{L}^2. \tag{49}$$

This expression coincides with (37) for $\mathcal{L}=0$, but it differs from the Taylor expansion of (35) for $\mathcal{L}\neq 0$. This means that $\mathcal{E}_{\min}$ is a nonanalytical function of κ and $\mathcal{L}$ at the point $\kappa=\mathcal{L}=0$, since the form of function $\mathcal{E}_{\min}(\kappa,\mathcal{L})$ depends on the sign of the difference $\kappa-\mathcal{L}$.

IV. PROPERTIES OF HIGHLY MIXED ROTATING THERMAL PACKETS

A. Covariance matrix and statistical operator

The equality $\eta=0$ implies the equalities $\xi=\alpha_{12}^{+}=0$: see Eq. (B3). Therefore $\alpha_{11}^{+}=\alpha_{22}^{+}=g_*$. Moreover, Eq. (28) shows that the ratio $(\mathcal{L}g-\gamma)^2/\eta^2$ is proportional to η^2, so that it tends to 0 when $\eta^2\to 0$. We deduce also from Eq. (B3) that $\Lambda=-\mathcal{L}\eta^2$, so that Eq. (B4) yields $\chi_{12}=-\xi\mathcal{L}=0$ in the case involved. This equality results in two other equalities: $\chi_{11}=\chi_{22}=0$. Equation (B1) shows that $\chi=\mathcal{L}\alpha_{12}^{+}$ for $\gamma=g\mathcal{L}$, therefore $\chi=0$ as well. This means that highly mixed minimal energy Gaussian states are described by the matrices A and B,

$$A=(g_*/2)(1+\mathcal{P}^{-1})I_2, \tag{50}$$

$$B=(g_*/2)[(1-\mathcal{P}^{-1})I_2+2i\mathcal{L}J_2], \tag{51}$$

where

$$J_2=\begin{Vmatrix}0&1\\-1&0\end{Vmatrix}. \tag{52}$$

The corresponding set of covariances between coordinates and momenta is

$$\overline{x^2} = \overline{y^2} = \overline{p_x^2} = \overline{p_y^2} = (2g_*)^{-1} = \mathcal{E}/2, \tag{53}$$

$$\overline{xp_y} = -\overline{yp_x} = \mathcal{L}/2, \tag{54}$$

$$\overline{xp_x} = \overline{yp_y} = \overline{xy} = \overline{p_x p_y} = 0, \tag{55}$$

so that the 4 × 4 covariance matrix, (10), has the following block form:

$$\mathcal{M} = \frac{1}{2}\left\| \begin{matrix} \mathcal{E}I_2 & -\mathcal{L}J_2 \\ \mathcal{L}J_2 & \mathcal{E}I_2 \end{matrix} \right\|. \tag{56}$$

The inverse covariance matrix reads

$$\mathcal{M}^{-1} = 2\mathcal{P}\left\| \begin{matrix} \mathcal{E}I_2 & \mathcal{L}J_2 \\ -\mathcal{L}J_2 & \mathcal{E}I_2 \end{matrix} \right\|. \tag{57}$$

Here $\mathcal{E}$ is the minimal energy given by Eq. (35).

The knowledge of the covariance matrix enables us to calculate the corresponding Gaussian statistical operator

$$\hat{\rho}_{\min} = \mathcal{N}_\rho \exp(-\hat{\mathbf{q}}\mathcal{Q}\hat{\mathbf{q}}/2) \tag{58}$$

according to the formula [9,16,73]

$$\mathcal{Q} = 2\Omega^{-1}\tanh^{-1}(\Omega\mathcal{M}^{-1}/2), \tag{59}$$

where $\Omega = -i\Sigma$ is the antisymmetric matrix constructed from the commutators between operators $\hat{q}_\alpha$ and $\hat{q}_\beta$. Taking into account the structure of matrix

$$\mathcal{X} = \Omega\mathcal{M}^{-1}/2 = i\mathcal{P}\left\| \begin{matrix} \mathcal{L}J_2 & -\mathcal{E}I_2 \\ \mathcal{E}I_2 & \mathcal{L}J_2 \end{matrix} \right\|, \tag{60}$$

one can see that matrix $Y = \tanh^{-1}(\mathcal{X})$ has a similar structure:

$$Y = \frac{i}{2}\left\| \begin{matrix} vJ_2 & -uI_2 \\ uI_2 & vJ_2 \end{matrix} \right\|. \tag{61}$$

To find the coefficients u and v, we note that matrix $\mathcal{X}$ has four real eigenvalues $\pm X_\pm$, where

$$X_\pm = \mathcal{P}(\mathcal{E} \pm \mathcal{L}) > 0 \tag{62}$$

(the eigenvalues of matrix $\mathcal{M}\Omega^{-1}$ nowadays are frequently called the symplectic eigenvalues of the covariance matrix [19,24–27], although their importance was understood much earlier [9–12]). Consequently, there exists the representation $\mathcal{X} = SX_dS^{-1}$, where S is some nonsingular matrix and X_d the diagonal matrix with elements $\pm X_\pm$. Therefore $Y = S\tanh^{-1}(X_d)S^{-1}$. Then the relation $\det(Y) = \det[\tanh^{-1}(X_d)]$ yields the equation

$$(u^2 - v^2)^2 = 16(\Lambda_+\Lambda_-)^2, \tag{63}$$

where

$$\Lambda_\pm = \tanh^{-1}(X_\pm) = \tanh^{-1}(\mathcal{P}[\mathcal{E} \pm \mathcal{L}]). \tag{64}$$

The equality $\mathrm{Tr}(Y^2) = \mathrm{Tr}[\tanh^{-1}(X_d)]^2$ yields the second equation,

$$v^2 + u^2 = 2(\Lambda_+^2 + \Lambda_-^2). \tag{65}$$

The admissible solutions to Eqs. (63) and (65) read (correct signs of u and v can be determined by taking into account the form of matrix Y in the limit case of $\mathcal{L} \to 0$)

$$u = \Lambda_+ + \Lambda_- = \tanh^{-1}(2\mathcal{P}\mathcal{E}/[1 + \mathcal{P}]), \tag{66}$$

$$v = \Lambda_+ - \Lambda_- = \tanh^{-1}(2\mathcal{P}\mathcal{L}/[1 - \mathcal{P}]). \tag{67}$$

Finally, we obtain

$$\mathcal{Q} = \left\| \begin{matrix} uI_2 & vJ_2 \\ -vJ_2 & uI_2 \end{matrix} \right\|, \tag{68}$$

$$\hat{\rho}_{\min} = \mathcal{N}_\rho \exp(-u\hat{H} + v\hat{L}_z). \tag{69}$$

Since operator (69) commutes with the Hamiltonian operator $\hat{H}$, (22), $\hat{\rho}_{\min}$ does not depend on time. It is noteworthy that the statistical operator, (69), is Hermitian, provided coefficients u and v are real. This condition means that the arguments of two $\tanh^{-1}$ functions in Eqs. (66) and (67) do not exceed unity in absolute value. One can easily check that this requirement results in inequality (36). This observation clarifies the physical meaning of condition (36).

Operator (69) has the same form as the equilibrium Gibbs statistical operator [74],

$$\hat{\rho}_{\mathrm{eq}} = \tilde{\mathcal{N}}_\rho \exp(-\beta[\hat{H} - \Omega\hat{\mathbf{L}}]), \tag{70}$$

where β is the inverse absolute temperature and Ω the angular velocity. This observation justifies the name *rotational thermal state*, attributed to state (69). In the special case of two-dimensional Gaussian states, we may thus identify $u = \beta$ and $\Omega = v/u$. However, parameter Ω has no direct physical meaning in this case, since the Gaussian packet does not rotate as a rigid body.

The statistical operator, (69), is diagonal in the energy – angular momentum basis $|n_r,m\rangle$, determined by the relations [75]

$$\hat{H}|n_r,m\rangle = (1 + |m| + 2n_r)|n_r,m\rangle, \tag{71}$$

$$\hat{L}_z|n_r,m\rangle = m|n_r,m\rangle, \tag{72}$$

with $n_r = 0, 1, 2, \ldots$ and $m = 0, \pm1, \pm2, \ldots$. Obviously,

$$\langle n_r,m|\hat{\rho}_{min}|n_r,m\rangle = \mathcal{N}_\rho \exp[-u(1+|m|+2n_r)+vm]. \tag{73}$$

Using (73) one can calculate the normalization coefficient,

$$\mathcal{N}_\rho = 4\sinh(\Lambda_+)\sinh(\Lambda_-). \tag{74}$$

B. Energy and angular momentum fluctuations

It would be interesting to know the values of the energy and angular momentum variances

$$\sigma_E \equiv \langle\hat{H}^2\rangle - \langle\hat{H}\rangle^2 = \langle m^2\rangle - \langle|m|\rangle^2 + 4\big(\langle n_r^2\rangle - \langle n_r\rangle^2\big), \tag{75}$$

$$\sigma_L \equiv \langle\hat{L}_z^2\rangle - \langle\hat{L}_z\rangle^2 = \langle m^2\rangle - \langle m\rangle^2. \tag{76}$$

We have taken into account that the matrix elements, (73), are factorized with respect to the quantum numbers n_r and m, so that $\langle n_r|m|\rangle = \langle n_r\rangle\langle|m|\rangle$. The average values contained in Eqs. (75) and (76) can be calculated with the aid of the generating function (dependent on the auxiliary variables x

and y)

$$G(x,y)=\sum_{n_r=0}^{\infty}\sum_{m=-\infty}^{\infty} x^{n_r}y^{m}\langle n_r,m|\hat{\rho}_{min}|n_r,m\rangle. \tag{77}$$

Separating sums over positive and negative values of the angular momentum projection m and using the identity $\tanh^{-1}(x)\equiv\frac{1}{2}\ln[(1+x)/(1-x)]$, we can write

$$G(x,y)=G_0 f(x)[1+F_+(y)+F_-(y)], \tag{78}$$

where

$$f(x)=(\varepsilon_+\varepsilon_- - x)^{-1},\quad G_0=(\varepsilon_+-1)(\varepsilon_- -1), \tag{79}$$

$$F_+(y)=(y^{-1}\varepsilon_- -1)^{-1},\quad F_-(y)=(y\varepsilon_+ -1)^{-1}, \tag{80}$$

$$\varepsilon_\pm=\exp(2\Lambda_\pm)=\frac{1+\mathcal{P}(\mathcal{E}\pm\mathcal{L})}{1-\mathcal{P}(\mathcal{E}\pm\mathcal{L})}. \tag{81}$$

It is important that the series in (77) are convergent and formulas (79) and (80) make sense in some vicinity of points $x=1$ and $y=1$. The probabilities of discovering 0, positive, and negative values of m are as follows:

$$p_0=G_0 f(1)=\mathcal{E}^{-1},\quad p_\pm=p_0F_\pm(1)=\frac{\mathcal{E}-1\pm\mathcal{L}}{2\mathcal{E}}. \tag{82}$$

In particular, $F_0\equiv 1+F_+(1)+F_-(1)=\mathcal{E}$, in accordance with the normalization condition $G(1,1)=1$. Calculating the first- and second-order derivatives of $G(x,y)$ at $x=y=1$, one obtains the following mean values:

$$\langle n_r\rangle=G_0F_0f'(1)=(1+\mathcal{P}-2\mathcal{P}\mathcal{E})/(4\mathcal{P}\mathcal{E}), \tag{83}$$

$$\langle m\rangle=G_0f(1)[F_+'(1)+F_-'(1)]=\mathcal{L}, \tag{84}$$

$$\langle|m|\rangle=G_0f(1)[F_+'(1)-F_-'(1)]=[\mathcal{E}^2+\mathcal{L}^2-1]/(2\mathcal{E}). \tag{85}$$

Combinations of the second- and first-order derivatives yield the second-order statistical moments:

$$\begin{aligned}\langle m^2\rangle&=G_0f(1)[F_+''(1)+F_+'(1)+F_-''(1)+F_-'(1)]\\&=\tfrac{1}{2}(\mathcal{E}^2+3\mathcal{L}^2-1),\end{aligned} \tag{86}$$

$$\langle n_r^2\rangle=G_0F_0[f''(1)+f'(1)]=\frac{(1+\mathcal{P})(1+\mathcal{P}-2\mathcal{P}\mathcal{E})}{8\mathcal{P}^2\mathcal{E}^2}. \tag{87}$$

Therefore

$$\sigma_L=\tfrac{1}{2}(\mathcal{E}^2+\mathcal{L}^2-1)=\mathcal{L}^2+\tfrac{1}{2}(\mathcal{P}^{-1}-1)\geqslant\mathcal{L}^2+|\mathcal{L}|, \tag{88}$$

$$\sigma_E=\mathcal{L}^2+\tfrac{1}{2}(\mathcal{P}^{-1}-1)=\sigma_L. \tag{89}$$

It is interesting that fluctuations of the angular momentum can be quite large in highly mixed states, even if $\mathcal{L}=0$. Another interesting observation is the identity of angular momentum and energy variances [normalized by $\hbar^2$ and $(\hbar\omega)^2$, respectively, in the dimensional variables].

C. Inhomogeneous Gaussian packets

The most general Gaussian packet is described by the Wigner function, (12), with nonzero mean value vector $\langle\mathbf{q}\rangle$. Representing quadrature operators as sums of average and fluctuating parts, e.g., $\hat{x}=x_0+\tilde{x}$, $\hat{p}_x=p_{x0}+\tilde{p}_x$, and so on, we can split the mean values of the angular momentum and energy operators into *classical* and *quantum* (or *intrinsic*) parts:

$$\begin{aligned}&\mathcal{L}=\mathcal{L}_c+\mathcal{L}_i,\quad \mathcal{E}=\mathcal{E}_c+\mathcal{E}_i,\\&\mathcal{L}_c=x_0p_{y0}-y_0p_{x0},\quad \mathcal{L}_i=\overline{xp_y}-\overline{yp_x},\\&\mathcal{E}_c=\tfrac{1}{2}\big(p_{x0}^2+p_{y0}^2+x_0^2+y_0^2\big),\quad \mathcal{E}_i=\tfrac{1}{2}\big(\overline{p_x^2}+\overline{p_y^2}+\overline{x^2}+\overline{y^2}\big).\end{aligned}$$

It is crucial that the mean values $\mathcal{L}_c$ and $\mathcal{L}_i$ are totally independent for Gaussian packets, as well as the quantities $\mathcal{E}_c$ and $\mathcal{E}_i$. Moreover, $\mathcal{L}_c$ and $\mathcal{E}_c$ do not depend on the quantum purity $\mathcal{P}$. The minimal value of $\mathcal{E}_i$ for fixed $\mathcal{L}_i$ was found in the preceding section. The minimization of the classical energy $\mathcal{E}_c$ for a fixed value of the classical angular momentum $\mathcal{L}_c$ is straightforward: $\mathcal{E}_c^{(\min)}(\mathcal{L}_c)=|\mathcal{L}_c|$. The minimizing trajectories of the packet center are circles, $x_0^2+y_0^2=|\mathcal{L}_c|$. To find the minimal energy with the fixed *total* mean angular momentum $\mathcal{L}$, one has to minimize the sum $\mathcal{E}=|\mathcal{L}_c|+\mathcal{E}_i^{\min}(\mathcal{L}-\mathcal{L}_c)$ with respect to the variable $\mathcal{L}_c$. If $2|\mathcal{L}-\mathcal{L}_c|<\mathcal{P}^{-1}-1$, then $\mathcal{E}(\mathcal{L}_c)=|\mathcal{L}_c|+[\mathcal{P}^{-1}+(\mathcal{L}-\mathcal{L}_c)^2]^{1/2}$, and it is easy to see that the minimum of this function is achieved for $\mathcal{L}_c=0$, i.e., for homogeneous Gaussian packets with $\langle\mathbf{q}\rangle=0$. However, we cannot claim that this is the most general answer, since we do not know the explicit form of the function $\mathcal{E}_i^{\min}(\mathcal{L}-\mathcal{L}_c)$ if $2|\mathcal{L}-\mathcal{L}_c|>\mathcal{P}^{-1}-1$. In particular, we know that there is a great degeneracy of the minimizing packets with respect to the decomposition of $\mathcal{L}$ into the sum of $\mathcal{L}_c$ and $\mathcal{L}_i$ in the case of pure states with $\mathcal{P}=1$ [69].

V. AN ISOTROPIC CHARGED OSCILLATOR IN A HOMOGENEOUS MAGNETIC FIELD

A two-dimensional isotropic oscillator in a homogeneous magnetic field B is described by the Hamiltonian (in the circular gauge of the vector potential and Gaussian units)

$$\hat{H}=\frac{\hat{\mathbf{p}}^2}{2M}+\frac{M\tilde{\omega}^2}{2}\hat{\mathbf{r}}^2-\omega_L\hat{L}_z, \tag{90}$$

$$\omega_L=\frac{eB}{2Mc},\quad \tilde{\omega}^2=\omega^2+\omega_L^2. \tag{91}$$

Obviously, minimal energy highly mixed *homogeneous* Gaussian packets with the fixed value $\langle\hat{L}_z\rangle=\hbar\mathcal{L}$ have the same form as those obtained in Sec. III, so that (we return here to dimensional variables)

$$\mathcal{E}_{\min}=\hbar\tilde{\omega}[\mathcal{P}^{-1}+\mathcal{L}^2]^{1/2}-\hbar\omega_L\mathcal{L} \tag{92}$$

under condition (36). In particular, the energy of a free particle ($\omega=0$) assumes the minimal (ground-state) value $\hbar\omega_L$ for all states with $\mathcal{L}\geqslant 0$ and the critical value of the purity $\mathcal{P}^{-1}=1+2\mathcal{L}$ (here we assume $\omega_L>0$).

The variance of the angular momentum is given by Eq. (88) for any values of $\tilde{\omega}$ and ω_L. The energy variance can be calculated in the same way as in Sec. IV B. But the result is different from (89), due to the form of the energy spectrum in the magnetic field [76]:

$$E_{n_r m}=\hbar\tilde{\omega}(1+|m|+2n_r)-\hbar\omega_L m. \tag{93}$$

In particular, we now need the additional second-order moment

$$\begin{aligned}\langle m|m|\rangle &= G_0 f(1)[F''_+(1) + F'_+(1) - F''_-(1) - F'_-(1)]\\ &= \mathcal{L}(3\mathcal{E}^2 + \mathcal{L}^2 - 1)/(2\mathcal{E}).\end{aligned} \tag{94}$$

The new result is

$$\begin{aligned}\sigma_E/\hbar^2 \; &= \big(\tilde{\omega}^2 + \omega_L^2\big)[\mathcal{L}^2 + (\mathcal{P}^{-1} - 1)/2]\\ &\quad - 2\tilde{\omega}\omega_L \mathcal{L}\sqrt{\mathcal{L}^2 + \mathcal{P}^{-1}}.\end{aligned} \tag{95}$$

In particular, for a free particle with $\omega_L \geqslant 0$ we have

$$\sigma_E/(\hbar\omega_L)^2 = (\sqrt{\mathcal{L}^2 + \mathcal{P}^{-1}} - \mathcal{L})^2 - 1, \tag{96}$$

so that $\sigma_E = 0$ in critical states with $\mathcal{L} \geqslant 0$ and $\mathcal{P}^{-1} = 1 + 2\mathcal{L}$. This happens due to the well-known infinite degeneracy of energy levels of a free charged particle moving in a homogeneous magnetic field.

VI. DISCUSSION

We have studied the statistical properties of specific mixed two-dimensional homogeneous Gaussian packets possessing the minimal energy for a fixed mean value of the angular momentum $\mathcal{L}$. Explicit analytical expressions have been obtained under the restriction $\mathcal{P}^{-1} \geqslant 1 + 2|\mathcal{L}|$, where $\mathcal{P}$ is the purity of the quantum state. We have shown that such packets can be interpreted as rotating thermal states. Some generic properties of two-dimensional Gaussian density matrices in the coordinate representation were discovered, especially the positivity condition, (21). However, answers to many questions are still to be found. One of them is: What happens if $\mathcal{P}^{-1} < 1 + 2|\mathcal{L}|$? It seems that the dependence $\mathcal{E}_{\min}(\mathcal{P})$ is not monotonous for a fixed value of $\mathcal{L}$. Indeed, $\mathcal{E}_{\min} = 1 + |\mathcal{L}|$ for $\mathcal{P} = 1$, whereas $\mathcal{E}_{\min}(\mathcal{P}) > 1 + |\mathcal{L}|$ for $0 < 1 - \mathcal{P} \ll 1$, according to Eq. (48). But $\mathcal{E}_{\min}(\mathcal{P}) = 1 + |\mathcal{L}|$ again if $\mathcal{P}^{-1} = 1 + 2|\mathcal{L}|$. Also, the question of the minimal energy of rotating inhomogeneous packets remains open in the most general case. A more challenging problem would be to try to find *non-Gaussian* minimal energy states with a fixed value of the mean angular momentum.

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APPENDIX A: EXPLICIT EXPRESSIONS FOR THE ELEMENTS OF THE GENERIC COVARIANCE MATRIX $\mathcal{M}$

The (co)variances of the coordinate and momentum operators in the mixed state, described by the Gaussian density matrix, (1), are as follows:

$$\overline{x^2} = \frac{\alpha_{22}^+}{2\Delta}, \quad \overline{y^2} = \frac{\alpha_{11}^+}{2\Delta}, \quad \overline{xy} = -\frac{\alpha_{12}^+}{2\Delta},$$

$$\overline{p_x x} = \frac{1}{2\Delta}(\chi_+\alpha_{12}^+ - \chi_{11}\alpha_{22}^+),$$

$$\overline{p_y y} = \frac{1}{2\Delta}(\chi_-\alpha_{12}^+ - \chi_{22}\alpha_{11}^+),$$

$$\overline{p_x y} = \frac{1}{2\Delta}(\chi_{11}\alpha_{12}^+ - \chi_+\alpha_{11}^+),$$

$$\overline{p_y x} = \frac{1}{2\Delta}(\chi_{22}\alpha_{12}^+ - \chi_-\alpha_{22}^+),$$

$$\overline{p_x^2} = \frac{1}{2\Delta}\big(\alpha_{11}^-\Delta + \chi_{11}^2\alpha_{22}^+ + \chi_+^2\alpha_{11}^+ - 2\chi_{11}\chi_+\alpha_{12}^+\big),$$

$$\overline{p_y^2} = \frac{1}{2\Delta}\big(\alpha_{22}^-\Delta + \chi_{22}^2\alpha_{11}^+ + \chi_-^2\alpha_{22}^+ - 2\chi_{22}\chi_-\alpha_{12}^+\big),$$

$$\begin{aligned}\overline{p_x p_y} = \frac{1}{2\Delta}[&\alpha_{12}^-\Delta + \chi_{11}\chi_-\alpha_{22}^+ + \chi_{22}\chi_+\alpha_{11}^+\\ &- \alpha_{12}^+(\chi_{11}\chi_{22} + \chi_+\chi_-)].\end{aligned}$$

The coefficients in these expressions are defined by Eqs. (4)–(6) and

$$\chi_\pm = \chi_{12} \pm \gamma. \tag{A1}$$

APPENDIX B: DETAILS OF THE MINIMIZATION PROCEDURE

Looking at function (23), one can conclude that the natural first step in its minimization is to minimize the function $f(\chi_{jk})$, (24), with respect to its arguments. In view of the structure of the right-hand side of Eq. (25), it is convenient to introduce the notation

$$\chi_{11} = z + \chi, \quad \chi_{22} = z - \chi,$$
$$\alpha_{11}^+ + \alpha_{22}^+ = 2g, \quad \alpha_{11}^+ - \alpha_{22}^+ = 2\xi.$$

Then we resolve Eq. (25) with respect to χ,

$$\chi = (\xi\chi_{12} + g\gamma - \mathcal{L}\Delta)/\alpha_{12}^+, \tag{B1}$$

and put (B1) into (24), arriving, after some algebra, at the function

$$\begin{aligned}f(z,\chi_{12}) &= \frac{2(g\alpha_{12}^+ z + \xi\Lambda - \eta^2\chi_{12})^2}{g(\alpha_{12}^+)^2} + \frac{2\Delta(\xi\Lambda - \eta^2\chi_{12})^2}{g\eta^2(\alpha_{12}^+)^2}\\ &\quad + \frac{2\Delta}{\eta^2}(g\mathcal{L}^2\Delta + g\gamma^2 - 2\gamma\mathcal{L}\Delta),\end{aligned} \tag{B2}$$

where

$$\Lambda = \mathcal{L}\Delta - g\gamma, \quad \eta^2 = \xi^2 + (\alpha_{12}^+)^2, \quad \Delta \equiv g^2 - \eta^2. \tag{B3}$$

Function (B2) has a minimum at

$$z = 0, \quad \chi_{12} = \xi\Lambda/\eta^2, \tag{B4}$$

so that we arrive at the function (using the relations $\alpha_{jj}^- = \alpha_{jj}^+ - 2b_{jj}$)

$$2\mathcal{E} = g(1 - \mathcal{L}^2) + \frac{g}{\Delta} + \frac{g}{\eta^2}(\mathcal{L}g - \gamma)^2 + 2\gamma\mathcal{L} - b_{11} - b_{22}. \tag{B5}$$

We want to find the minimum of this function under the additional restriction, (9), which can be written as

$$\begin{aligned}R(b_{jk}) \equiv \Delta^{-1}\big[&b_{11}b_{22} - b_{12}^2 + \alpha_{12}^+ b_{12}\\ &- (\alpha_{11}^+ b_{22} + \alpha_{22}^+ b_{11})/2\big] = \kappa,\end{aligned}$$

where the nonnegative parameter κ is defined in Eq. (29). Using the parametrization $\xi = \eta\cos(\varphi)$, $\alpha_{12}^+ = \eta\sin(\varphi)$, we can write

$$R(b_{jk}) = \Delta^{-1}\big[b_{11}b_{22} - b_{12}^2 - g(b_{11}+b_{22})/2 + \eta\sin(\varphi)b_{12} + \eta\cos(\varphi)(b_{11}-b_{22})/2\big].$$

Now we can use the Lagrange multiplier method and look for the extremum of function

$$f = 2\mathcal{E} + \lambda R(b_{jk}) \tag{B6}$$

with respect to the independent variables g, η, b_{jk}, and φ, considering γ as a free parameter (for a while) and λ as the Lagrange multiplier. First, we look for the extremum of f with respect to phase φ, arriving at the function

$$R(b_{jk}) = \Delta^{-1}\big[b_{11}b_{22} - b_{12}^2 - g(b_{11}+b_{22})/2 \pm (\eta/2)\sqrt{(b_{11}-b_{22})^2 + 4b_{12}^2}\big]. \tag{B7}$$

The equations $\partial f/\partial b_{jk} = 0$ have the following solutions:

$$b_{12} = 0, \quad b_{11} = b_{22} = g/2 + \Delta/\lambda. \tag{B8}$$

Putting these solutions into (B7), one can see that condition (B6) leads to the equality

$$\kappa\Delta = b_{11}^2 - gb_{11} = (\Delta/\lambda)^2 - g^2/4,$$

so that

$$\Delta/\lambda = \pm\tfrac{1}{2}\sqrt{g^2 + 4\kappa\Delta}.$$

The parameter λ must be negative, in order to fulfill the condition $b_{11} = 0$ at $\kappa = 0$. Therefore we find

$$b_{11} = b_{22} = -\frac{2\kappa\Delta}{g + \sqrt{g^2 + 4\kappa\Delta}}. \tag{B9}$$

Equation $\partial f/\partial\eta = 0$ can be reduced to the form (using the relation $\Delta = g^2 - \eta^2$ and setting the value of λ after the differentiation)

$$\frac{g\eta}{\Delta^2} - \frac{g(\mathcal{L}g - \gamma)^2}{\eta^3} - \frac{2\kappa\eta}{\sqrt{g^2 + 4\kappa\Delta}} = 0. \tag{B10}$$

The equation $\partial f/\partial g = 0$ reads

$$\frac{g(1+4\kappa)}{\sqrt{g^2+4\kappa\Delta}} + \frac{1}{\eta^2}[\mathcal{L}^2\Delta + 2(\mathcal{L}g-\gamma)^2 - \gamma^2] = \frac{g^2+\eta^2}{\Delta^2}. \tag{B11}$$

Excluding $(\mathcal{L}g - \gamma)^2$ from Eqs. (B10) and (B11), we get Eq. (27). Getting rid of the denominator η^3 in (B10), we arrive at Eq. (28). Then formula (26) follows from Eqs. (B5), (B9), and (28).

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