

Variational approximations in a path integral description of potential scattering

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Abstract. Using a recent path integral representation for the \mathcal{T} -matrix in nonrelativistic potential scattering we investigate new variational approximations in this framework. By means of the Feynman-Jensen variational principle and the most general ansatz quadratic in the velocity variables —over which one has to integrate functionally— we obtain variational equations which contain classical elements (trajectories) as well as quantum-mechanical ones (wave spreading). We analyse these equations and solve them numerically by iteration, a procedure best suited at high energy. The first correction to the variational result arising from a cumulant expansion is also evaluated. Comparison is made with exact partial-wave results for scattering from a Gaussian potential and better agreement is found at large scattering angles where the standard eikonal-type approximations fail.

1 Introduction

Variational approaches to quantum-mechanical scattering have a long history and are well covered in standard text books (*e.g.* [1–4]). Actually, as formulated in ref. [5], it is “... possible to construct systematically a variational principle for just about any given quantity of interest, provided that the entities which enter into the definition of (that quantity) are uniquely defined by a set of equations ...”. For quantum physics the observables obtained from a solution of Schrödinger’s equation are of particular interest and therefore variational principles have been available since the beginning of quantum mechanics. Best known is the Rayleigh-Ritz variational principle for the ground-state energy of bound systems but the continuous spectrum is also accessible to a variational treatment. Most prominent among the variational principles for scattering are Schwinger’s [6] and Kohn’s [7] expressions. In particular, Kohn’s variational principle is widely used in nuclear [8–10] and atomic [11,12] physics for an approximate description of few-body scattering near thresholds.

While these approaches benefit from the flexibility which ingenious trial wave functions offer it is well known that in many-body systems or in field theory the use of *wave functions* (or functionals) ceases to be useful. The path integral method where one integrates functionally over the degrees of freedom weighted by the exponential

of the classical *action* is much more general although the cases where one can actually perform the path integral are rare. Therefore, in general, one has to resort to approximations, such as perturbation theory or brute-force numerical evaluation of the functional integral on a (space-time) lattice. If this is not appropriate or feasible, one may use a variational principle extended to actions. A prime example is the Feynman-Jensen variational principle which has been used to obtain the best semi-analytic ground-state energy of an electron in an ionic crystal (the polaron problem [13]).

Oddly enough, scattering has mostly remained outside the path integral approach and it is only at zero energy that bounds for the scattering length have been obtained from the path integral in the imaginary-time formulation [14,15]. Expanding on previous attempts [16] a real-time path integral representation for the nonrelativistic \mathcal{T} -matrix in potential scattering has recently been derived [17]. In this formulation the particle travels mainly along a simple reference path while quantum fluctuations around this path are taken into account by functional integration over velocities. It has been shown that this description gives the exact Born series to all orders if an expansion in powers of the potential is done and reduces to the eikonal approximation (valid at high energies and small scattering angles) when the quantum fluctuations are neglected altogether. Taylor-expanding the action around the reference path and performing the Gaussian functional integrations term by term, a variant of the systematic eikonal expansion of the scattering amplitude derived by Wallace [18] is obtained (higher orders have

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been calculated in ref. [19]). This is very promising for applications to many-body scattering as the eikonal approximation is the basis of Glauber's very successful theory of high-energy scattering from composite targets [20,21].

Given this affinity to a geometric description of high-energy scattering and the success of Feynman's treatment of the polaron problem it seems interesting to study how a variational approach to potential scattering performs in this framework. With a simple (linear) *ansatz* for the trial action this has been investigated in ref. [22] where it was found that the classical trajectory —and not a straight-line path as in the eikonal approximation— determines the scattering dynamics¹. Numerically, very promising results in potential scattering have been obtained in cases where the eikonal expansion fails.

It is the purpose of the present work to generalize this work by allowing for the most general *quadratic + linear* trial action. One may expect that the additional quadratic term describes the wave-spreading characteristic for the exact quantum theory thus leading to a much better description of the scattering process.

To be in agreement with the high-energy eikonal expansion such an *ansatz* must allow for anisotropic terms which have already been shown to improve a variational calculation in a scalar field theory [24]. Since the Feynman-Jensen variational principle is the first term of a cumulant expansion it is also possible to calculate systematic corrections. We do it here by evaluating the second cumulant which is similar as in the polaron problem [25,26] but also more challenging as we have to deal with the complex scattering amplitude.

The paper is organized as follows: in sect. 2 we present the essentials of the path integral representations of the \mathcal{T} -matrix in potential scattering so that we can apply the Feynman-Jensen variational principle in this setting. Section 3 contains the variational *ansatz* and derives the ensuing variational equations. Some properties of the solutions and special cases are then discussed and the correction by the second cumulant is given. Section 4 then presents our numerical results for high-energy scattering from a Gaussian potential and comparison with exact partial-wave calculation of the scattering amplitude as well with other approximations discussed in the literature. The work concludes with a summary and outlook for further work and application. Most of the technicalities as calculation of various path integral averages and numerical details are collected in four appendices.

2 Path integral representations of the scattering amplitude

Recently two variants of a path integral representation for the \mathcal{T} -matrix in potential scattering have been given [17] in the form

$$\mathcal{T}_{i \rightarrow f} = i \frac{K}{m} \int d^2b e^{-i\mathbf{q} \cdot \mathbf{b}} [S(\mathbf{b}) - 1], \quad (2.1)$$

¹ Corrections to the straight-line trajectory also have turned out to be important in heavy-ion collisions [23].

where

$$\mathbf{K} = \frac{1}{2} (\mathbf{k}_i + \mathbf{k}_f), \quad K \equiv |\mathbf{K}| = k \cos \frac{\theta}{2}, \quad (2.2)$$

$$\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i, \quad q \equiv |\mathbf{q}| = 2k \sin \frac{\theta}{2} \quad (2.3)$$

are the mean momentum and momentum transfer, respectively. $k^2/(2m)$ is the scattering energy (we set $\hbar = 1$) and θ the scattering angle. For lack of a better nomenclature we will call $S(\mathbf{b})$ the “impact-parameter \mathcal{S} -matrix” although eq. (2.1) is *not* a strict impact-parameter representation of the scattering amplitude. This is because of the dependence of $S(\mathbf{b})$ on additional kinematic variables like \mathbf{K} or \mathbf{q} which we do not show explicitly and the angle-dependent factor $K = k \cos(\theta/2)$ in front of the impact-parameter integral: in a genuine impact-parameter representation all dependence on the scattering angle θ should only reside in the factor $\exp(-i\mathbf{q} \cdot \mathbf{b})$ [27].

The main features of these representations are functional integration over velocities without boundary conditions and the use of “phantom” degrees of freedom to get rid of explicit phases which would diverge in the limit of large scattering times. Two versions exist which are distinguished by the reference path along which the particle dominantly travels and the dimensionality d of the “anti-velocity” $\mathbf{w}(t)$ which is needed to achieve the cancellation²:

$$S(\mathbf{b}) = \int \mathcal{D}^3v \mathcal{D}^d w \exp \left\{ i \int_{-\infty}^{+\infty} dt \frac{m}{2} [\mathbf{v}^2(t) - \mathbf{w}^2(t)] \right\} \times \exp \left\{ i \chi(\mathbf{b}, \mathbf{v}, \mathbf{w}) \right\}, \quad (2.4a)$$

$$\chi(\mathbf{b}, \mathbf{v}, \mathbf{w}) = - \int_{-\infty}^{+\infty} dt V(\mathbf{x}_{\text{ref}}(t) + \mathbf{x}_{\text{quant}}(t, \mathbf{v}, \mathbf{w})). \quad (2.4b)$$

In the first case the reference path is a straight-line path along the mean momentum

$$\mathbf{x}_{\text{ref}}^{(d=3)}(t) = \mathbf{b} + \frac{\mathbf{K}}{m} t \quad (2.5)$$

and the quantum fluctuations are given by

$$\mathbf{x}_{\text{quant}}^{(d=3)}(t, \mathbf{v}, \mathbf{w}) = \mathbf{x}_v(t) - \mathbf{x}_w(0) \quad (2.6)$$

where

$$\mathbf{x}_v(t) = \frac{1}{2} \int_{-\infty}^{+\infty} dt' \text{sgn}(t-t') \mathbf{v}(t'), \quad \dot{\mathbf{x}}_v(t) = \mathbf{v}(t) \quad (2.7)$$

and $\text{sgn}(x) = 2\Theta(x) - 1$ is the sign function. We will call that the “aikonal” representation because it gives rise to the eikonal approximation of Abarbanel and Itzykson (AI) [28] if the quantum fluctuations are neglected altogether.

² The path integrals are normalized such that $S(\mathbf{b}) \equiv 1$ for zero potential. Our notation indicates that χ is a function of \mathbf{b} but a functional of $\mathbf{v}(t)$ and $\mathbf{w}(t)$. Similarly for $\mathbf{x}_{\text{quant}}$.

In the second case the anti-velocity is only 1-dimensional and the reference path is a *ray* along the initial momentum for $t < 0$ and along the final momentum for $t > 0$

$$\begin{aligned}\mathbf{x}_{\text{ref}}^{(d=1)}(t) &= \mathbf{b} + \left[\hat{\mathbf{k}}_i \Theta(-t) + \hat{\mathbf{k}}_f \Theta(t) \right] \frac{k}{m} t \\ &= \mathbf{b} + \frac{\mathbf{K}}{m} t + \frac{\mathbf{q}}{2m} |t|\end{aligned}\quad (2.8)$$

and the quantum fluctuations are given by

$$\mathbf{x}_{\text{quant}}^{(d=1)}(t, \mathbf{v}, w) = \mathbf{x}_v(t) - \mathbf{x}_{\perp v}(0) - \hat{\mathbf{K}} x_{\parallel}(0). \quad (2.9)$$

We will call that the “ray” representation in the following.

For further details we refer to ref. [17]. Here we just note that systematic eikonal-like expansions can be obtained by Taylor-expanding the potential around the reference path

$$\begin{aligned}\chi(\mathbf{b}, \mathbf{v}, \mathbf{w}) &= - \int_{-\infty}^{+\infty} dt \left[V(\mathbf{x}_{\text{ref}}) + \mathbf{x}_{\text{quant}} \cdot \nabla V(\mathbf{x}_{\text{ref}}) \right. \\ &\quad \left. + \frac{1}{2} (\mathbf{x}_{\text{quant}})_i (\mathbf{x}_{\text{quant}})_j \partial_i \partial_j V(\mathbf{x}_{\text{ref}}) + \dots \right]\end{aligned}\quad (2.10)$$

and performing successively the functional (Gaussian) integrations over velocity and anti-velocity. This is because a simple scaling argument shows that each quantum fluctuation $\mathbf{x}_{\text{quant}}$ is suppressed by a power of $1/\sqrt{K}$ in the case of the “aikonal” representation or $1/\sqrt{k}$ in the “ray” representation. Therefore at high energy/small scattering angle the geometrical (classical) picture of scattering is dominant.

3 Variational calculation

3.1 The Feynman-Jensen variational principle

Being highly nonlinear in velocity and anti-velocity variables the path integrals in eq. (2.4a) cannot be performed analytically in general³. Numerical methods or approximations are then necessary. For weak potentials, for example, one may expand in powers of the potential and it has been shown that the Born series for the \mathcal{T} -matrix is obtained in all orders [17]. At high energy and small scattering angles eikonal approximations are useful. Because a variational approach neither requires weak interaction nor high energy, forward scattering it is widely used in atomic and molecular physics, mostly in the form of Kohn’s variational principle [7]. Schwinger’s functional is also stationary against variation of trial wave *functions* [6] but more difficult to use in practice.

³ It would be interesting to derive the few exact expressions for scattering amplitudes of a local potential which are available in the quantum-mechanical literature, *e.g.* for the Coulomb potential.

The path integral representation (2.4a) immediately suggests another variational approximation for the *action*

$$\begin{aligned}\mathcal{A}[\mathbf{v}, \mathbf{w}] &= \int_{-\infty}^{+\infty} dt \left[\frac{m}{2} (\mathbf{v}(t)^2 - \mathbf{w}(t)^2) \right. \\ &\quad \left. - V\left(\mathbf{x}_{\text{ref}}(t) + \mathbf{x}_{\text{quant}}(t, \mathbf{v}, \mathbf{w})\right) \right],\end{aligned}\quad (3.1)$$

viz the Feynman-Jensen variational principle. For a positive weight function this principle employs the convexity of $\exp(-x)$ to obtain the inequality

$$\langle e^{-\Delta\mathcal{A}} \rangle_t \geq e^{-\langle \Delta\mathcal{A} \rangle_t} \quad (3.2)$$

but in real time (in which scattering occurs) one only has stationarity:

$$\begin{aligned}S(\mathbf{b}) &= \int \mathcal{D}^3 v \mathcal{D}^d w \frac{e^{i\mathcal{A}_t} \int \mathcal{D}^3 v \mathcal{D}^d w \exp(i\mathcal{A}_t + i\mathcal{A} - i\mathcal{A}_t)}{\int \mathcal{D}^3 v \mathcal{D}^d w \exp(i\mathcal{A}_t)} \\ &\stackrel{\text{stat}}{\sim} S_t(\mathbf{b}) \cdot e^{i\langle \Delta\mathcal{A} \rangle_t}, \quad \Delta\mathcal{A} \equiv \mathcal{A} - \mathcal{A}_t,\end{aligned}\quad (3.3)$$

where

$$\langle \Delta\mathcal{A} \rangle_t := \frac{\int \mathcal{D}^3 v \mathcal{D}^d w \Delta\mathcal{A} \exp(i\mathcal{A}_t)}{\int \mathcal{D}^3 v \mathcal{D}^d w \exp(i\mathcal{A}_t)} \quad (3.4)$$

is the average of the difference between the full action \mathcal{A} and the trial action \mathcal{A}_t weighted with the oscillating factor $\exp(i\mathcal{A}_t)$. Note that both Kohn’s and Schwinger’s variational principles also are only stationary when applied to the full \mathcal{T} -matrix. This seems inevitable when trying to estimate a complex quantity by variational means; only for real quantities, like a scattering length, a minimum principle is available (see Chapt. 11.3.4 in ref. [4]).

3.2 Variational ansatz and equations

As usual in variational calculations the outcome crucially depends on the test functions/actions which must lead to expressions which may be evaluated safely. Unfortunately in the path integral formalism one is restricted to trial actions which are at most *quadratic* in the dynamical variables so that the various path integrals and averages can be worked out analytically. This restricts somewhat the utility of this approach which —on the other hand— is so general that it can be applied not only for the scattering of a single particle in quantum mechanics but also in the many-body case or even in field theory. In the present case it means that our trial action \mathcal{A}_t may contain linear and at most quadratic terms in the velocity *and* the anti-velocity. So we may take

$$\begin{aligned}\mathcal{A}_t[\mathbf{v}, \mathbf{w}] &= \int_{-\infty}^{+\infty} dt dt' \frac{m}{2} \left[\mathbf{v}(t) A_{vv}(t, t') \mathbf{v}(t') \right. \\ &\quad + \mathbf{w}(t) A_{ww}(t, t') \mathbf{w}(t') \\ &\quad + \mathbf{v}(t) A_{vw}(t, t') \mathbf{w}(t') \\ &\quad \left. + \mathbf{w}(t) A_{wv}(t, t') \mathbf{v}(t') \right] \\ &\quad + \int_{-\infty}^{+\infty} dt \left[\mathbf{B}_v(t) \cdot \mathbf{v}(t) + \mathbf{B}_w(t) \cdot \mathbf{w}(t) \right]\end{aligned}\quad (3.5)$$

since constant terms cancel out in the Feynman-Jensen variational principle. Special cases are the free action and the *ansatz* studied in ref. [22] where only the \mathbf{B} -terms were varied while the quadratic part was left as in the free case.

At this stage it is useful to have a look at the high-energy expansion in eq. (2.10): it tells us that the functions A_{vv} , A_{ww} , A_{vw} , A_{wv} have to be *anisotropic* in order to describe the high-energy expansion up to and including terms of order $1/K^2$ (in the “aikonal” representation) or $1/k^2$ in the “ray” representation. Thus the various variational functions $A_{vv}(t, t')$... actually are 3×3 matrices in cartesian space if the most general quadratic trial action is considered. Similar anisotropic trial actions have already been considered in a variational description of world-line scalar field theory [24] and shown to give considerable improvement. A slight complication here is the presence of the anti-velocity which, however, can be elegantly handled by grouping it together with the velocity to form a $(3 + d)$ -dimensional “super-vector”

$$\mathbb{V}^{(3-3)} = \begin{pmatrix} \mathbf{v} \\ \mathbf{w} \end{pmatrix}, \quad \text{or} \quad \mathbb{V}^{(3-1)} = \begin{pmatrix} \mathbf{v} \\ \mathbf{w}_{\parallel} \end{pmatrix} \quad (3.6)$$

so that the trial action can be written succinctly as

$$\mathbb{A}_t = \frac{m}{2} \mathbb{V} \cdot \mathbb{A} \mathbb{V} + \mathbb{B} \cdot \mathbb{V}. \quad (3.7)$$

Here \mathbb{B} is a $(3 + d)$ -dimensional vector made up of the variational functions $\mathbf{B}(t)$

$$\mathbb{B} = \begin{pmatrix} \mathbf{B}_v \\ \mathbf{B}_w \end{pmatrix} \quad (3.8)$$

and \mathbb{A} a $(3 + d) \times (3 + d)$ -dimensional symmetric matrix formed by the variational (3×3) -matrix functions $A(t, t')$

$$\mathbb{A} = \begin{pmatrix} A_{vv} & A_{vw} \\ A_{wv} & A_{ww} \end{pmatrix}. \quad (3.9)$$

In eq. (3.7) we employ a nomenclature where also the integration over continuous times is treated like a summation over identical indices. See appendix A for a more detailed account of our conventions. This allows to evaluate the various path integrals and averages in an efficient way and to derive the variational equations easily as detailed in appendix B.

Here we just collect the final results: after variation the stationary value of the impact-parameter \mathcal{S} -matrix reads

$$S_{\text{var}}(\mathbf{b}) = \exp[i(X_0 + X_1) - \Omega], \quad (3.10)$$

where

$$X_0 \equiv \langle \chi \rangle_t = - \int_{-\infty}^{+\infty} dt V_{\sigma(t)}(\boldsymbol{\rho}(t)), \quad (3.11)$$

$$X_1 = \frac{1}{2} \int_{-\infty}^{+\infty} dt dt' \partial_i V_{\sigma}(t)(\boldsymbol{\rho}(t)) (\Sigma_0)_{ij}(t, t') \times \partial_j V_{\sigma(t')}(t') \equiv \frac{1}{2} J_{\sigma}^T \Sigma_0 J_{\sigma} \quad (3.12)$$

are “phases” and

$$\Omega = \frac{1}{2} \text{Tr} \left[-\text{Ln} (1 + \Sigma H_{\sigma}) + \Sigma H_{\sigma} \right]. \quad (3.13)$$

is the “fluctuation term” (or an imaginary phase) which arises from the functional determinant due to the quadratic term in our *ansatz*. “Tr” denotes the trace both in continuous and discrete variables and “T” the transpose of a vector or a matrix. Actually, the terminology used above is a little bit misleading as it turns out that all these quantities become complex. This is because they are not determined by the real potential and its derivatives but by its Gaussian transforms with a *complex* width $\sigma(t)$ (see below). This entails that different branches of the multi-valued logarithmic function “Ln” may be needed depending on the appropriate sign of the square root of the *complex* functional determinant. These subtleties of the complex Gaussian integral which require a “branch tracking” are discussed in appendix D.4.

The Gaussian transform of the potential is most conveniently defined in momentum space as

$$\begin{aligned} \tilde{V}_{\sigma(t)}(\mathbf{p}) &:= \tilde{V}(\mathbf{p}) \exp \left[-\frac{1}{2} \mathbf{p}^T \sigma(t) \mathbf{p} \right] \\ &= \tilde{V}(\mathbf{p}) \exp \left[-\frac{1}{2} p_i \sigma_{ij}(t) p_j \right], \end{aligned} \quad (3.14)$$

and we can form the Jacobian (the vector of derivatives)

$$(J_{\sigma})_i := \partial_i V_{\sigma} \quad (3.15)$$

and the Hessian (the matrix of second derivatives)

$$(H_{\sigma})_{ij} := \partial_i \partial_j V_{\sigma}. \quad (3.16)$$

They are functions of a trajectory $\boldsymbol{\rho}_{\text{var}}(t)$ (we will omit the subscript “var” in the following) which is determined by the following equation of motion

$$\boldsymbol{\rho}_{\text{var}}(t) = \mathbf{x}_{\text{ref}}(t) + \int_{-\infty}^{+\infty} dt' \Sigma_0(t, t') \mathbf{J}_{\sigma(t')}(\boldsymbol{\rho}_{\text{var}}(t')). \quad (3.17)$$

Here we encounter the (3×3) -matrix Σ_0 which in the “aikonal” representation takes the form

$$\Sigma_0^{(3-3)}(t, t') = -\frac{1}{2m} |t - t'| \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (3.18)$$

whereas in the “ray” representation it reads

$$\Sigma_0^{(3-1)}(t, t') = -\frac{1}{2m} \begin{pmatrix} d(t, t') & 0 & 0 \\ 0 & d(t, t') & 0 \\ 0 & 0 & |t - t'| \end{pmatrix} \quad (3.19a)$$

with

$$d(t, t') = |t - t'| - |t| - |t'| \quad (3.19b)$$

if the mean momentum \mathbf{K} is chosen to be along the 3-direction. Finally, it is found that the time-dependent width of the Gaussian transform

$$\sigma(t) = i \Sigma(t, t) \quad (3.20)$$

is proportional to the diagonal part of a matrix Σ which fulfills a Lippmann-Schwinger-like equation

$$\Sigma = \Sigma_0 + \Sigma_0 H_\sigma \Sigma. \quad (3.21)$$

In contrast to the familiar Lippmann-Schwinger equation in scattering theory this is a *nonlinear* equation since the Gaussian width of the potential and its Hessian depends on the diagonal part of Σ . Note that eq. (3.21) holds for both representations and that all dependence on the phantom degrees of freedom has now disappeared. In particular, no divergences are encountered for large scattering times—the job for which the anti-velocity was introduced in the beginning. We find it also remarkable that in the final outcome the variational functions \mathbb{A} , \mathbb{B} whose physical interpretation is not immediately evident are replaced by the trajectory $\boldsymbol{\rho}$ and the Green function Σ which have a clear classical and quantum-mechanical meaning.

Equations (3.17), (3.21) and (3.20) form a system of coupled variational equations which have to be solved. Once that is done we may insert the solutions into the variational functional to get the impact-parameter \mathcal{S} -matrix (3.10).

3.3 Correction by the second cumulant

It is possible to calculate systematic corrections to the variational result (or improving the variational principle) by realizing that the Feynman-Jensen variational principle is the first term of a *cumulant expansion*

$$\langle e^{i\Delta\mathcal{A}} \rangle_t = \exp \left[i\lambda_1 + \frac{i^2}{2!} \lambda_2 + \dots \right], \quad (3.22)$$

where

$$\lambda_1 = \langle \Delta\mathcal{A} \rangle_t \quad (3.23)$$

is just what enters the Feynman-Jensen variational principle and

$$\lambda_2 = \langle (\Delta\mathcal{A})^2 \rangle_t - \langle \Delta\mathcal{A} \rangle_t^2 \quad (3.24)$$

the first correction to it. So the variational functional becomes

$$S_{\text{var+cum}}(\mathbf{b}) = \exp \left[i(X_0 + X_1) - \Omega - \frac{1}{2} \lambda_2 \right]. \quad (3.25)$$

In principle one could vary the full functional with respect to the variational functions/parameters but we follow the standard practice to add the second cumulant as a correction [25] with the parameters fixed by the Feynman-Jensen variational principle, *i.e.* the first cumulant. This allows to use the variational equations for these parameters and leads to a considerable simplification of the final expression.

Appendix C gives the result of evaluating the second cumulant in our case:

$$\lambda_2 = \langle \chi^2 \rangle_t - \langle \chi \rangle_t^2 - iJ_\sigma^T \Sigma J_\sigma + \frac{1}{2} \text{Tr}(\Sigma H_\sigma)^2, \quad (3.26)$$

where

$$\begin{aligned} \langle \chi^2 \rangle_t &= \int_{-\infty}^{+\infty} dt_1 dt_2 \int \frac{d^3 p_1 d^3 p_2}{(2\pi)^6} \tilde{V}(\mathbf{p}_1) \tilde{V}(\mathbf{p}_2) \\ &\times \exp \left\{ -\frac{i}{2} (\mathbf{p}_1^T, \mathbf{p}_2^T) \begin{pmatrix} \Sigma(t_1, t_1) & \Sigma(t_1, t_2) \\ \Sigma(t_2, t_1) & \Sigma(t_2, t_2) \end{pmatrix} \begin{pmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \end{pmatrix} \right. \\ &\left. + i(\mathbf{p}_1^T, \mathbf{p}_2^T) \begin{pmatrix} \boldsymbol{\rho}(t_1) \\ \boldsymbol{\rho}(t_2) \end{pmatrix} \right\} \end{aligned} \quad (3.27)$$

involves a double Gaussian transform of the squared potential. All other quantities have been defined and calculated before in both representations. It is easy to see that $\Delta\mathcal{A}$ is of first (and higher) order in the potential. By construction the n -th cumulant then contains contributions of $\mathcal{O}(V^n)$ and higher. This implies that the second Born approximation to the \mathcal{T} -matrix is fully included in our calculation when the second cumulant is added.

3.4 A special case: the linear ansatz

A less general variational *ansatz* has been made in ref. [22] by only allowing the linear terms in the trial action to vary whereas the quadratic part was fixed to be the free action. In the present nomenclature this amounts to setting $\mathbb{A} = \sigma_3$. Inspecting the variational solution for \mathbb{A} we see that the results of ref. [22] should be recovered by setting the Hessian of the potential to zero: $H_\sigma \rightarrow 0$. Indeed, then the solution of the Lippmann-Schwinger eq. (3.21) simply is $\Sigma = \Sigma_0$ and the Gaussian width becomes

$$\sigma_{ij}(t) \Big|_{\text{linear}} = -\frac{i|t|}{m} \delta_{ij} \begin{cases} 0, & \text{“aikonal”}, \\ (1 - \delta_{i3}), & \text{“ray”}. \end{cases} \quad (3.28)$$

Thus in the “aikonal” case (with a 3-dimensional anti-velocity) there is no Gaussian transform of the potential and the variational equation for the trajectory simply is

$$\boldsymbol{\rho}(t) = \mathbf{b} + \frac{K}{m} t - \frac{1}{2m} \int_{-\infty}^{+\infty} dt' |t - t'| \nabla V(\boldsymbol{\rho}(t')) \quad (3.29)$$

which, after differentiating twice, is just Newton’s law for the classical motion in the potential:

$$\ddot{\boldsymbol{\rho}}(t) = -\frac{1}{m} \nabla V(\boldsymbol{\rho}(t)). \quad (3.30)$$

However, the boundary conditions encoded in the integral eq. (3.29) are unusual: using $|t - t'| \rightarrow |t - \text{sgn}(t)t'|$ for large $|t|$ one finds from eq. (3.29)

$$\begin{aligned} \boldsymbol{\rho}(t) &\xrightarrow{t \rightarrow \pm\infty} \left[\frac{\mathbf{K}}{m} \mp \int_{-\infty}^{+\infty} dt' \frac{\mathbf{J}(t')}{2m} \right] t + \mathbf{b} \pm \int_{-\infty}^{+\infty} dt' t' \frac{\mathbf{J}(t')}{2m} \\ &+ \text{terms which vanish for } |t| \rightarrow \infty, \end{aligned} \quad (3.31)$$

so that

$$\lim_{T \rightarrow \infty} \{ \boldsymbol{\rho}(T) + \boldsymbol{\rho}(-T) - T[\dot{\boldsymbol{\rho}}(T) - \dot{\boldsymbol{\rho}}(-T)] \} = 2\mathbf{b}, \quad (3.32a)$$

$$\lim_{T \rightarrow \infty} \{ \dot{\boldsymbol{\rho}}(T) + \dot{\boldsymbol{\rho}}(-T) \} = 2 \frac{\mathbf{K}}{m}. \quad (3.32b)$$

It is the great advantage of the integration over velocities that the boundary conditions are exactly built in and we do not have to worry about them during (approximate) evaluation of the path integral. Note that the boundary conditions (3.32a) and (3.32b) are just those needed to convert an integral equation with the kernel $|t - t'|$ into a differential equation [29].

For the linear *ansatz* in the “aikonal” representation the trajectories are real and consequently the phases X_0 and X_1 are also real; an imaginary phase, *i.e.* a real part in $\ln S(\mathbf{b})$ only develops due the second cumulant. It is easily seen that the general expression (3.27) for λ_2 reduces to the eq. (4.84) in ref. [22], if Σ is replaced by $\Sigma_0^{(3-3)}$. As usual one finds from Newton’s equation (3.30) the conservation law $m\dot{\boldsymbol{\rho}}^2(t)/2 + V(\boldsymbol{\rho}(t)) = \mathcal{E} = \text{const}$. Inserting the asymptotic behaviour (3.31) and using the symmetry of the solutions under $t \rightarrow -t$ which forces $\int_{-\infty}^{+\infty} dt' \mathbf{J}(\mathbf{t}')$ to be perpendicular to the mean momentum \mathbf{K} , the conserved quantity is

$$\mathcal{E} = \frac{\mathbf{K}^2}{2m} + \frac{1}{8m} \left(\int_{-\infty}^{+\infty} dt' \mathbf{J}(\mathbf{t}') \right)^2 \quad (3.33)$$

which means that this “energy” depends on the impact parameter \mathbf{b} . This is because $S(\mathbf{b}) = S(\mathbf{b}, \mathbf{K})$ does not contain any information on the actual scattering energy

$$\frac{k^2}{2m} = \frac{\mathbf{K}^2}{2m} + \frac{\mathbf{q}^2}{8m}. \quad (3.34)$$

However, the variational principle is “clever” enough to mimic the missing term as good as possible:

$$\mathbf{q} \simeq - \int_{-\infty}^{+\infty} dt' \nabla_b V(\boldsymbol{\rho}(t')) \quad (3.35)$$

is what one would obtain if the impact-parameter integral over $\exp(iX_0)$ is evaluated by a saddle-point approximation.

Things are slightly different in the “ray” representation: first, the potential is replaced by its Gaussian transform with an anisotropic width given in eq. (3.28) which renders it complex from the very beginning. Second, the anisotropic kernel (3.19a) leads to an equation of motion where the particle experiences a kick at $t = 0$ and the “energy” of that motion is not conserved anymore during the scattering process but only asymptotically (see fig. 1 in ref. [22]). Complex trajectories are frequently encountered in semi-classical approximations of quantum motion in regions of space which are forbidden classically. In our variational approximations, however, the main reason for this behaviour (which shows up even above any potential hill) is unitarity: $S(\mathbf{b})$ cannot be unimodular [18].

We do not dwell on several other interesting properties of our variational approximation with a linear *ansatz* but refer to ref. [22] for more details.

3.5 High-energy expansion

By construction the variational solution of the quadratic + linear variational *ansatz* (3.7) must contain the high-

energy expansion (2.10). To show how that comes out we will take here for simplicity the “aikonal” representation as the algebra in the “ray” representation is more involved.

First, we switch to distances instead of times by defining

$$z := \frac{K}{m} t \Rightarrow t = \frac{m}{K} z. \quad (3.36)$$

We then see that

$$\Sigma_0^{(3-3)}(z, z') = -\frac{1}{2K} |z - z'| \quad (3.37)$$

is suppressed for large energies and forward scattering angles (recall $K = k \cos(\theta/2)$) since the arguments z, z' are bounded by the range of the potential. We thus may expand in powers of Σ_0 and obtain from the Lippmann-Schwinger-like eq. (3.21)

$$\Sigma = \Sigma_0 + \Sigma_0 H_\sigma \Sigma_0 + \dots \quad (3.38)$$

Equation (3.20) then gives for the Gaussian width

$$\sigma_{ij}(z) = \frac{i}{(2K)^2} \int_{-\infty}^{+\infty} dz' |z - z'|^2 \frac{m}{K} (H_{\sigma(z')})_{ij}(z') + \dots, \quad (3.39)$$

as the first-order term vanishes in the “aikonal” representation (this is not the case in the “ray” representation!). Therefore the Gaussian width becomes also small under these kinematical conditions (note that m/K does not need to be small) so that H_σ may be replaced by H up to order $1/K^2$. From the definition (3.14) of the Gaussian transform we find

$$V_{\sigma(z)}(\boldsymbol{\rho}(z)) = V(\boldsymbol{\rho}(z)) + \frac{1}{2} \sigma_{ij}(z) H_{ij}(\boldsymbol{\rho}(z)) + \dots \quad (3.40)$$

and iterating the equation of motion (3.17) one obtains

$$\boldsymbol{\rho} = \mathbf{x}_{\text{ref}} + \Sigma_0 \mathbf{J} + \Sigma_0 H \Sigma_0 \mathbf{J} + \dots \quad (3.41)$$

Here and in the following the potential, the Jacobian and the Hessian are all evaluated with the straight-line reference path $\mathbf{x}_{\text{ref}}(z) = \mathbf{b} + \hat{K}z$. Inserting these expressions into eqs. (3.11)–(3.13), and expanding up to order $1/K^2$ we get in our short-hand notation

$$X_0 \rightarrow \chi_{\text{AI}}^{(0)} - J^T \Sigma_0 J - \frac{3}{2} J^T \Sigma_0 H \Sigma_0 J - \frac{i}{2} \text{Tr}(\Sigma_0 H)^2, \quad (3.42)$$

$$X_1 \rightarrow \frac{1}{2} J^T \Sigma_0 J + J^T \Sigma_0 H \Sigma_0 J, \quad (3.43)$$

$$\Omega \rightarrow \frac{1}{4} \text{Tr}(\Sigma_0 H)^2, \quad (3.44)$$

where

$$\chi_{\text{AI}}^{(0)} = - \int_{-\infty}^{+\infty} dt V(\mathbf{x}_{\text{ref}}(t)) = -\frac{m}{K} \int_{-\infty}^{+\infty} dz V(\mathbf{b} + \hat{K}z) \quad (3.45)$$

is the standard eikonal phase from Abarbanel and Itzykson [28]. We see that

$$X_0 + X_1 \rightarrow \chi_{\text{AI}}^{(0)} + \chi_{\text{AI}}^{(1)} + \chi_{\text{AI}}^{(2)} + 2i \omega_{\text{AI}}^{(2)} + \mathcal{O}\left(\frac{1}{K^3}\right), \quad (3.46)$$

where in our condensed notation

$$\chi_{\text{AI}}^{(1)} = -\frac{1}{2} J^T \Sigma_0 J, \quad \chi_{\text{AI}}^{(2)} = -\frac{1}{2} J^T \Sigma_0 H \Sigma_0 J, \quad (3.47)$$

$$\omega_{\text{AI}}^{(2)} = -\frac{1}{4} \text{Tr}(\Sigma_0 H)^2 \quad (3.48)$$

are exactly the first- and second-order corrections to the leading ‘‘aikonal’’ result as given in eqs. (4.97), (4.103) and (4.110) of ref. [22]. Note that the contribution (3.44) from the fluctuation term brings the imaginary part into full agreement⁴ with what is needed for unitarity in the high-energy limit:

$$\text{Im}X_0 + \Omega \rightarrow 2\omega_{\text{AI}}^{(2)} - \omega_{\text{AI}}^{(2)} + \mathcal{O}\left(\frac{1}{K^3}\right) = \omega_{\text{AI}}^{(2)} + \mathcal{O}\left(\frac{1}{K^3}\right). \quad (3.49)$$

How is that high-energy behaviour changed by including the second cumulant? To answer this question we consider eq. (3.27) and decompose

$$\begin{pmatrix} \Sigma(t_1, t_1) & \Sigma(t_1, t_2) \\ \Sigma(t_2, t_1) & \Sigma(t_2, t_2) \end{pmatrix} = \frac{1}{i} \begin{pmatrix} \sigma(t_1) & 0 \\ 0 & \sigma(t_2) \end{pmatrix} + \begin{pmatrix} 0 & \Sigma(t_1, t_2) \\ \Sigma(t_2, t_1) & 0 \end{pmatrix} \quad (3.50)$$

into a diagonal and a nondiagonal part. The diagonal part is seen to convert the potentials into Gaussian transformed potentials while the nondiagonal part gives new contributions when the exponential is expanded:

$$\begin{aligned} \langle \chi^2 \rangle &= \langle \chi \rangle^2 + iJ^T \Sigma J + \frac{i^2}{2} \text{Tr}(H_\sigma \Sigma H_\sigma \Sigma) \\ &+ \frac{i^3}{6} \int_{-\infty}^{+\infty} dt_1 dt_2 (\partial_{2i} \Sigma(t_1, t_2)_{ij} \partial_{1j})^3 \\ &\times V_{\sigma(t_1)}(\boldsymbol{\rho}(t_1)) V_{\sigma(t_2)}(\boldsymbol{\rho}(t_2)) + \dots \end{aligned} \quad (3.51)$$

It is seen that the first 3 terms on the r.h.s. are completely cancelled when forming the second cumulant in eq. (3.26) and that in the high-energy limit the leading contribution comes from the last term involving 3 powers of the matrix Σ . In that limit we may safely replace it by the zeroth-order matrix Σ_0 so that the second cumulant gives an imaginary (phase) correction at $\mathcal{O}(1/K^3)$. It is interesting that in the linear approximation the last term in eq. (3.26) is absent and that the contribution $-\lambda_2/2$ from the second cumulant then correctly supplies the real term $\omega_{\text{AI}}^{(2)}$. In contrast, the more general, anisotropic quadratic + linear trial action already gives variational results correct up to and including $\mathcal{O}(1/K^2)$ as expected from the high-energy expansion. Similar results hold in the ‘‘ray’’ representation except that here the expansion parameter is the wave number k and not the mean momentum $K = k \cos(\theta/2)$.

⁴ To show that one has to convert to an impact-parameter representation of the scattering matrix for which the $K = k \cos(\theta/2)$ -factors in the ‘‘aikonal’’ representation give additional contributions. As they are the same as worked out in ref. [22] we do not have to consider them here.

3.6 A Feynman-Hellman theorem

Some further properties of the variational approximation for the impact-parameter \mathcal{S} -matrix (3.10) can be obtained by employing the variational equations in a particular way. This has already been used in a variational approximation to the relativistic bound-state problem [30] and is just a variant of the well-known Feynman-Hellmann theorem in quantum mechanics (see, *e.g.* refs. [31,32]).

Suppose there is some parameter λ in the potential or in the reference path. As the variational functional also depends on it implicitly via the variational parameters/functions \mathbb{A}_{var} and \mathbb{B}_{var} one may perform the differentiation with respect to this parameter by means of the chain rule⁵

$$\begin{aligned} \frac{\partial \ln S_{\text{var}}}{\partial \lambda} &= \frac{\partial \ln S_{\text{var}}}{\partial \mathbb{A}_{AB}^{\text{var}}} \frac{\partial \mathbb{A}_{AB}^{\text{var}}}{\partial \lambda} + \frac{\partial \ln S_{\text{var}}}{\partial \mathbb{B}_A^{\text{var}}} \frac{\partial \mathbb{B}_A^{\text{var}}}{\partial \lambda} \\ &- i \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial \lambda} V_{\sigma(t)}(\boldsymbol{\rho}(t)) \\ &= -i \int_{-\infty}^{+\infty} dt \frac{\partial}{\partial \lambda} V_{\sigma(t)}(\boldsymbol{\rho}(t)), \end{aligned} \quad (3.52)$$

since the first two terms vanish identically for the variational solutions \mathbb{A}_{var} and \mathbb{B}_{var} . This leads to a simple result although these solutions may be very complicated functions of the parameter λ .

As an example take the dependence of the impact-parameter \mathcal{S} -matrix on the mean momentum K in the ‘‘aikonal’’ representation. The sole explicit dependence of the variational functional resides in the reference path $\mathbf{x}_{\text{ref}}(t) = \mathbf{b} + \mathbf{K}t/m$. Therefore we immediately have the relation

$$\frac{\partial \ln S_{\text{var}}^{(3-3)}}{\partial K} = -\frac{i}{m} \hat{\mathbf{K}} \cdot \int_{-\infty}^{+\infty} dt t \nabla V_{\sigma(t)}(\boldsymbol{\rho}(t)). \quad (3.53)$$

Similarly, one obtains

$$\frac{\partial \ln S_{\text{var}}}{\partial b} = -i \hat{\mathbf{b}} \cdot \int_{-\infty}^{+\infty} dt \nabla V_{\sigma(t)}(\boldsymbol{\rho}(t)) \quad (3.54)$$

which also holds for the ‘‘ray’’ representation. Finally the dependence on the strength V_0 of the potential is given by the simple expression

$$V_0 \frac{\partial \ln S_{\text{var}}}{\partial V_0} = -i \int_{-\infty}^{+\infty} dt V_{\sigma(t)}(\boldsymbol{\rho}(t)) \equiv iX_0. \quad (3.55)$$

These relations may be used to derive or check high-energy or weak-coupling expansions by expanding the r.h.s. in powers of the particular parameter and integrating term by term.

⁵ Here it is important that only X_0 is assumed to depend explicitly on λ , whereas X_1, Ω do not. See eqs. (B.2), (B.3), (B.4) in appendix B. We use the short-hand notation of appendix A.

For example, using the first two terms of the high-energy expansion (3.41) we have in the “aikonal” representation

$$\hat{\mathbf{K}} \cdot \nabla V_{\sigma(t)}(\boldsymbol{\rho}(z)) = \frac{\partial}{\partial z} \left[V(\mathbf{x}_{\text{ref}}(z)) - \frac{1}{2K} \nabla V(\mathbf{x}_{\text{ref}}(z)) \cdot \int dz' |z - z'| \nabla V(\mathbf{x}_{\text{ref}}(z')) + \mathcal{O}(1/K^2) \right] \quad (3.56)$$

since the Gaussian width does not contribute in this order. Substituting this into the Feynman-Hellmann relation (3.53) (expressed in the z -variable to make $\mathbf{x}_{\text{ref}}(z)$ independent of K) and integrating with respect to K gives the correct result $\ln S_{\text{var}}^{(3-3)} = i\chi_{\text{AI}}^{(0)} + i\chi_{\text{AI}}^{(1)} + \mathcal{O}(1/K^3)$ if an integration by parts in z is performed.

In appendix D.6 we use the dependence (3.55) on the coupling strength as a nontrivial check for our numerical procedures to solve the variational equations.

3.7 Semi-classical expansion

It is of some interest to distinguish the present variational approach from the usual semi-classical approximation of the path integral propagator obtained by the stationary phase approximation (see, *e.g.* ref. [33], Chapt. 13 or ref. [34], Chapt. 4). To do that we have to restore the appropriate \hbar -factors in the path integral representation (2.4a). This is easily done by remembering that the weight in the path integral is always the exponential of $i \times$ the action divided by \hbar and that the velocities in the reference path are *momenta* ($= \hbar \times$ wave numbers) divided by the mass of the particle. To account for that we simply have to substitute

$$m \longrightarrow \frac{1}{\hbar} m, \quad (3.57)$$

$$V \longrightarrow \frac{1}{\hbar} V, \quad (3.58)$$

everywhere. From the explicit expressions (3.18) and (3.19a) we then see that

$$\Sigma_0 = \mathcal{O}(\hbar) \quad (3.59)$$

and from the Lippmann-Schwinger-like equation (3.21) that

$$\Sigma = \mathcal{O}(\hbar) + \text{higher orders in } \hbar \quad (3.60)$$

since eq. (3.58) also implies the multiplication of the Jacobian and Hessian by $1/\hbar$. In other words: the Gaussian width $\sigma(t) \equiv \Sigma(t, t)$ is a pure quantum effect which vanishes in the classical approximation. The “higher orders in \hbar ” in eq. (3.60) are generated by the nonlinearity of the Lippmann-Schwinger-like equation via the Gaussian transform of the Hessian H_σ . Similarly, the Gaussian transform of the Jacobian J_σ in eq. (3.17) gives rise to \hbar -dependent terms in the trajectory

$$\boldsymbol{\rho}_{\text{var}}(t) = \boldsymbol{\rho}_{\text{class}}(t) + \mathcal{O}(\hbar) + \dots, \quad (3.61)$$

where $\boldsymbol{\rho}_{\text{class}}(t)$ is the trajectory for zero Gaussian width. By the same arguments we see from eqs. (3.11), (3.12) that the phases

$$X_0, X_1 = \mathcal{O}\left(\frac{1}{\hbar}\right) + \mathcal{O}(\hbar^0) + \dots, \quad (3.62)$$

whereas from eq. (3.13) one finds that

$$\Omega = \mathcal{O}(\hbar^0) + \dots \quad (3.63)$$

Finally, applying the scaling laws (3.58) and (3.60) to eqs. (3.26), (3.27) we deduce that

$$\lambda_2 = \mathcal{O}(\hbar) + \dots \quad (3.64)$$

is a genuine quantum correction. We thus see that our variational approach is *not* equivalent to a semi-classical approximation as it contains (an infinite number of) \hbar -dependent terms. This is mostly due to the quadratic term in our general variational *ansatz* (3.7) which gives rise to an interaction-dependent Gaussian width: the more restricted linear *ansatz* studied in ref. [22] leads to a vanishing Gaussian width in the “aikonal” (3-3) representation; only in the “ray” (3-1) representation one obtains a nonzero width which generates some quantum corrections.

4 Numerical results

We compare our results with those of a (basically) exact partial-wave calculation of scattering from a Gaussian potential

$$V(r) = V_0 e^{-\alpha r^2} = V_0 e^{-r^2/R^2} \quad (4.1)$$

with parameters

$$\begin{aligned} 2mV_0R^2 &= -4, \\ kR &= 4. \end{aligned} \quad (4.2)$$

This was considered as a test case for the systematic eikonal expansion by Wallace in ref. [18] and (with $V_0 = -41.6$ MeV and $R = 1$ fm) used to describe phenomenologically the scattering of α -particles from α -particles at an energy of 166 MeV. We also choose it because for this potential a persistent failure of the eikonal expansion to describe the scattering at larger angles was observed: the scattering angle where the eikonal amplitude started to deviate appreciably increased only slightly when higher-order corrections were included (see fig. 6 in ref. [18]).

Thus, this particular potential is a good *litmus test* for checking any approximate description of high-energy scattering. However, we do not use

$$\frac{\Delta\sigma}{\sigma} := \frac{d\sigma/d\Omega|_{\text{approx}} - d\sigma/d\Omega|_{\text{exact}}}{d\sigma/d\Omega|_{\text{exact}}} \quad (4.3)$$

as the usual measure to gauge agreement/disagreement with the exact result but

$$\left| \frac{\Delta f}{f} \right| := \left| \frac{f_{\text{approx}} - f_{\text{exact}}}{f_{\text{exact}}} \right|. \quad (4.4)$$

Here

$$f(\theta) = -\frac{m}{2\pi} \mathcal{T}_{i \rightarrow f} \quad (4.5)$$

is the scattering amplitude and

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \quad (4.6)$$

the differential cross-section. By construction the quantity in eq. (4.4) also measures the *phase* deviation of the scattering amplitude f_{approx} from the exact amplitude. Indeed, if

$$f_{\text{exact}} = r e^{i\phi} \quad \text{and} \quad f_{\text{approx}} = (r + \Delta r) e^{i(\phi + \Delta\phi)} \quad (4.7)$$

then one finds to first order in the deviations Δr , $\Delta\phi$

$$\left| \frac{\Delta f}{f} \right| = \sqrt{(\Delta\phi)^2 + (\Delta r/r)^2} \quad (4.8)$$

and

$$\frac{\Delta\sigma}{\sigma} = 2 \frac{\Delta r}{r} \quad (4.9)$$

which is independent of the phase error $\Delta\phi$. As

$$\left| \frac{\Delta\sigma}{\sigma} \right| \leq 2 \left| \frac{\Delta f}{f} \right| \quad (4.10)$$

one may even encounter cases where $\Delta\sigma/\sigma = 0$ although $|\Delta f/f| \neq 0$ because the approximate scattering amplitude has the correct modulus but the wrong phase. So the common practice of comparing just differential cross-sections can be misleading.

Table 1 gives the values of the exact calculation obtained by integrating the Schrödinger equation for each partial wave up to a radius where the solution could be matched to a linear combination of free spherical waves. By varying this radius as well as the step size for the numerical integration and the number of partial waves retained we made sure that the numerical values given in this table are at least accurate to the number of digits given. We display scattering amplitude and differential cross-section in units of powers of R since the range of the potential sets the length scale.

4.1 Variational results

We have evaluated the coupled variational equations by an iterative scheme on a grid in time (more precisely: in distances which the particle travels while in the range of the potential) and then evaluated the phases X_0 , X_1 , the fluctuation term Ω and the second cumulant λ_2 . Some numerical details are given in appendix D.

In table 2 we list the relative deviation of the scattering amplitude for the various approximations from the exact partial-wave result as a function of the scattering angle θ . For the different variational approximations we use the

Table 1. Exact partial-wave amplitude and differential cross-section for scattering from the Gaussian potential (4.1) with $2mV_0R^2 = -4$ at $kR = 4$. Amplitude and cross-section are given in units of R and R^2 , respectively, where R is the range of the potential. The number in parenthesis indicates the power of ten by which the numerical value has to be multiplied, e.g. $5.6472(-6) \equiv 5.6472 \cdot 10^{-6}$.

θ [°]	$(\text{Re } f)/R$	$(\text{Im } f)/R$	$\frac{d\sigma}{d\Omega}/R^2$
0	1.7348 (0)	3.8758 (-1)	3.1596 (0)
5	1.6806 (0)	3.8172 (-1)	2.9702 (0)
10	1.5282 (0)	3.6466 (-1)	2.4683 (0)
15	1.3042 (0)	3.3788 (-1)	1.8151 (0)
20	1.0445 (0)	3.0358 (-1)	1.1831 (0)
25	7.8431 (-1)	2.6444 (-1)	6.8507 (-1)
30	5.5114 (-1)	2.2323 (-1)	3.5358 (-1)
35	3.6078 (-1)	1.8249 (-1)	1.6347 (-1)
40	2.1785 (-1)	1.4435 (-1)	6.8294 (-2)
45	1.1867 (-1)	1.1032 (-1)	2.6252 (-2)
50	5.5103 (-2)	8.1274 (-2)	9.6419 (-3)
55	1.7782 (-2)	5.7530 (-2)	3.6259 (-3)
60	-1.8100 (-3)	3.8913 (-2)	1.5175 (-3)
65	-1.0380 (-2)	2.4924 (-2)	7.2893 (-4)
70	-1.2687 (-2)	1.4870 (-2)	3.8207 (-4)
75	-1.1832 (-2)	7.9883 (-3)	2.0380 (-4)
80	-9.6765 (-3)	3.5396 (-3)	1.0616 (-4)
85	-7.2471 (-3)	8.6532 (-4)	5.3269 (-5)
90	-5.0442 (-3)	-5.8091 (-4)	2.5782 (-5)
95	-3.2623 (-3)	-1.2260 (-3)	1.2145 (-5)
100	-1.9307 (-3)	-1.3856 (-3)	5.6472 (-6)

following naming scheme:

$$\left. \begin{array}{l} \text{B 3d: variational } \textit{ansatz} \text{ with linear term } \mathbb{B} \\ \text{only [22],} \\ \text{Bc 3d: variational } \textit{ansatz} \text{ with linear term } \mathbb{B} \\ \text{+ second cumulant [22],} \\ \text{AB 3d: variational } \textit{ansatz} \text{ with quadratic} \\ \text{+ linear terms } \mathbb{A} \text{ and } \mathbb{B}, \\ \text{ABc 3d: variational } \textit{ansatz} \text{ with quadr. + linear} \\ \text{terms } \mathbb{A} \text{ and } \mathbb{B} \text{ + second cumulant.} \end{array} \right\} \quad (4.11)$$

where $d = 3$ (“aikonal”) or $d = 1$ (“ray”). Note that we list

$$10^4 \cdot \left| \frac{\Delta f}{f} \right| \quad (4.12)$$

which is necessary to show the rather small deviations of the scattering amplitude —any discrepancies in the cross-sections would not be seen on a logarithmic scale except at large scattering angles.

Two independent programs using different subroutines and (partially) different techniques have been developed and run to arrive at these results. Many checks have been

Table 2. The relative deviation (in units of 10^{-4}) of the scattering amplitude from the exact value for scattering from the Gaussian potential (4.1) with $2mV_0R^2 = -4$ at $kR = 4$. The variational approximations are labeled according to the scheme (4.11). The numbers in parenthesis give the estimated numerical error of the calculations in units of the last digit. Entries are stopped if the deviation exceeds 10%.

θ [°]	B 33	B 31	Bc 33	Bc 31	AB 33	AB 31	ABc 33	ABc 31
0	12	25	7	9	7	5	2	1
5	12	25	7	9	7	5	3 (1)	1
10	14	24	8	10	8	6	3 (1)	1
15	17	24	9	11	9	6	3 (1)	1
20	22	23	10	12	11	7	4 (1)	1
25	32	21	12	15	16	9	5 (1)	1
30	55	17	15	19	26	11	7 (1)	1
35	104	20	19	25	46	17	10 (1)	2
40	203	43	25	33	88	26	14 (1)	4
45	394	97	36	47 (1)	174	45	20 (1)	6 (1)
50	743	197	58	67 (2)	345	85	32 (3)	9 (2)
55	1307	362	101	86 (5)	657	161	47 (2)	15 (3)
60		593	180	105 (9)	1141	287	78 (2)	27 (5)
65		862	309	113 (15)		471	139 (2)	52 (4)
70		1152	509	108 (24)		725	255 (2)	91 (4)
75			822	102 (37)		1079	468 (4)	163 (9)
80			1320	135 (33)			856 (6)	280 (9)
85				275 (37)			1567 (10)	511 (17)
90				488 (54)				940 (44)

performed (see appendix D) including a test of the Feynman-Hellmann theorem for the interaction strength which is a highly nontrivial test of how well the variational equations are fulfilled. In addition, the various accuracy parameters have been varied to ensure stability of the numerical outcome. For the approximations including the second cumulant which demand particular care we also include in table 2 an approximate numerical error estimated from the different results from both programs and from variation of the integration parameters.

A systematic improvement is seen when quadratic terms and/or the correction by the second cumulant are included. This is shown in fig. 1 where the deviations of the different results for the scattering amplitude are plotted on a *linear* scale. We also have included the best result from the variational approximation with a linear ansatz plus the second cumulant (Bc 31). It is seen that including the second cumulant gives much improved results so that the variational approximations labelled Bc 31 and ABc 31 give the best overall results. However, at present we do not fully understand why at larger scattering angles the (much simpler) scheme Bc 31 outperforms the more involved scheme ABc 31 which includes the quantum-mechanical spreading effects. As we simply have added the second cumulant on top of the variational results and not used it in the variational optimization there is, of course, no guarantee that ABc 31 does *always* better than Bc 31 whereas AB 3d has always to be better or at least as good as B 3d⁶. It should also be noted that the evaluation of the second cumulant

⁶ Otherwise the variational principle would have chosen the free A as the best solution.

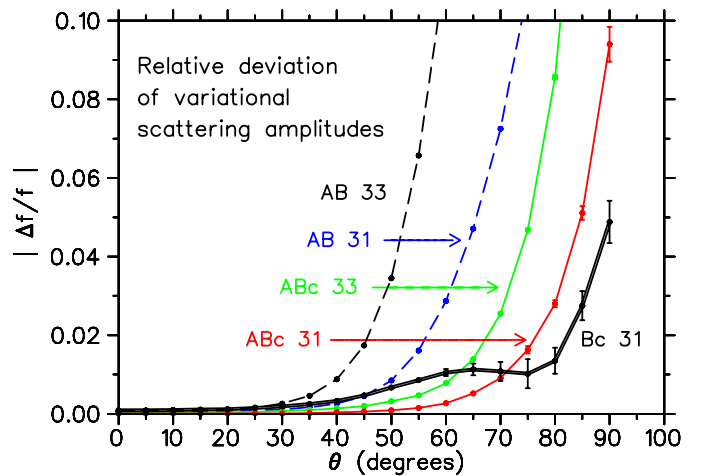


Fig. 1. (Color online) The relative deviation $|\Delta f/f|$ of the variational amplitudes from the exact scattering amplitude as function of the scattering angle θ . The naming scheme (4.11) is used for the various approximations.

at large scattering angles where the amplitude is down by many orders of magnitude is a very demanding numerical task and the numerical errors given in table 2 may be underestimated.

Nevertheless, the full “ray” approximation plus the second cumulant (ABc 31), for example, provides a very good approximation even at larger scattering angles: at $\theta = 90^\circ$ the complex scattering amplitude is reproduced within 9% and the cross-section to better than 2%

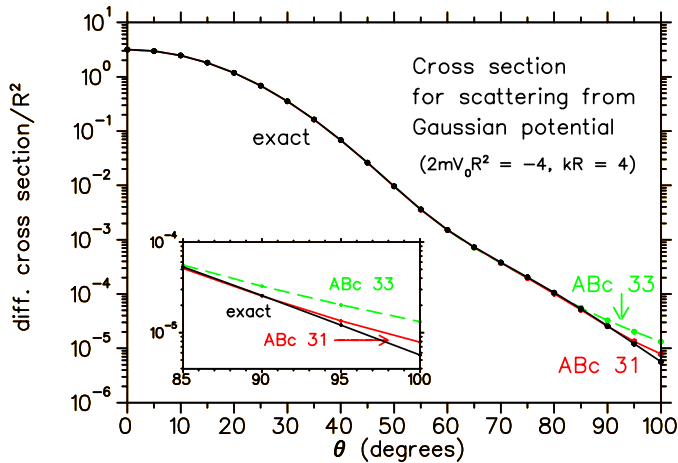


Fig. 2. (Color online) The exact cross-section for scattering from a Gaussian potential with strength $2mV_0R^2 = -4$ at $kR = 4$ and the best variational cross-sections including the second cumulant.

although the latter one is down by 5 orders of magnitude from the value taken in forward direction.

Only at large scattering angles the deviations from the exact partial-wave result again start to grow and become so large that they even can be seen on the usual logarithmic plot for the cross-section in fig. 2.

4.2 Comparison with other work

Combining the eikonal approximation with the second-order Born approximation Chen has proposed several approximations which should also work at larger scattering angles and which we denote by “Chen 1” [35], “Chen 2” [36] and “Chen 3” [37].

The relative deviation of his approximate amplitudes from the exact value has been calculated by direct numerical integration and is displayed in table 3 and fig. 3. It is seen that these approximations are clearly inferior to the present variational approximations although they use some analytic properties specific to the potential under consideration. In contrast, the variational approach requires as input just the (Gaussian transform of the) potential and thus can be applied more generally.

We also include the results for Wallace’s systematic eikonal expansion⁷ including real and imaginary phases up to second and third order in $1/k$. This makes for a relevant comparison with our variational results which have been shown to be correct up to second order in the high-energy expansion but contain many other higher-order terms.

Table 3 and fig. 3 show that these systematic expansions are very good in forward direction but fail at higher scattering angles. Again the variational approximations are clearly better in this kinematical regime.

⁷ For a Gaussian potential the explicit expressions are given in table I of ref. [18].

Table 3. Relative deviation (in units of 10^{-4}) of the scattering amplitude from the exact value for various approximations by Chen [35–37] and Wallace [18]. In the latter case the subscripts denote the order of the eikonal expansion which is included. The potential is again a Gaussian one with the same parameters as in table 2.

θ [°]	Chen 1	Chen 2	Chen 3	Wallace ₂	Wallace ₃
0	217	5	40	4	< 1
5	220	6	40	4	1
10	231	9	42	5	1
15	250	15	45	7	1
20	279	25	49	9	1
25	320	42	55	9	2
30	378	67	63	8	4
35	456	108	72	3	9
40	560	170	84	17	15
45	693	266	98	53	24
50	844	406	115	122	35
55	971	585	142	232	47
60	1001	767	194	376	66
65	891	907	281	528	110
70	672	999	405	678	192
75	400	1078	563	844	317
80	244	1190	765	1065	499
85	555	1390	1024	1392	763
90	1082	1739	1357	1898	1150

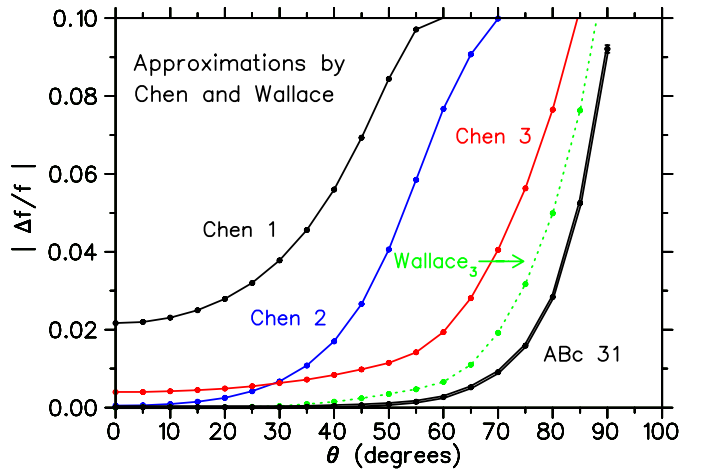


Fig. 3. (Color online) Same as in fig. 1 but for the various approximations by Chen and Wallace’s 3rd-order eikonal expansion. For comparison also the best variational result (ABc 31 in the naming scheme (4.11)) is shown.

5 Summary and outlook

We have applied the Feynman-Jensen variational principle to two variants of a new path integral representation of the T -matrix in potential scattering using the most general *trial action* which contains quadratic and linear terms both in velocity and anti-velocity. Merging these variables into a “super-velocity” the variational functional was easily derived and the variational equations immediately followed by demanding stationarity of that functional. As expected the anti-velocity (“phantom”) degrees of freedom

prevented any divergence to appear when the scattering time was sent to infinity as it should be when the initial and final states are detected in the scattering process.

We have found that this quadratic + linear *ansatz* describes the scattering in terms of a (nearly) classical trajectory $\rho(t)$ with peculiar boundary conditions and a matrix operator Σ which is the solution of a one-dimensional Lippmann-Schwinger-like equation. This reflects the classical as well as the quantum-mechanical (“wave spreading”) aspects of the process dominant in the high-energy, forward scattering and low-energy scattering regime, respectively. Unlike the previous linear *ansatz* [22] the present variational approach immediately leads to complex phases in the impact-parameter \mathcal{S} -matrix as required by unitarity and a fluctuation term coming from the corresponding functional determinant. We were also able to evaluate the first correction (the second cumulant) in a systematic cumulant expansion.

As we solved the nonlinear, coupled variational equations iteratively (both in analytic and numerical evaluations) the present work is mostly devoted to the high-energy case with “wave-spreading” corrections becoming more important at backward scattering angles. Indeed we have seen better and better agreement with exact partial-wave calculations of scattering from a Gaussian potential as we step from the linear trial action to the quadratic + linear and from the version which uses a straight-line reference path and a 3-dimensional anti-velocity (“aikonal” or “3-3”) to the version with a ray-like reference path and a 1-dimensional anti-velocity (“ray” or “3-1”). An even more dramatic improvement is obtained if the correction by the second cumulant is added because then the second-order Born approximation is contained in the variational result—an observation also made by Chen (refs. [35–37]). Instead of plotting the approximate cross-sections on a logarithmic scale as is usually done, we give the numerical values for the relative deviation of the approximate scattering amplitudes from the exact partial-wave result. This is done for a particular benchmark case: scattering from a Gaussian potential with fixed parameters (4.2) and allows a *quantitative* comparison of the different approaches for a case where large-angle scattering has been notoriously difficult to describe.

We also have shown analytically that in a high-energy expansion terms up to inverse second order in k or $K = k \cos(\theta/2)$ for “ray” or “aikonal” representation are correctly reproduced. Thus our variational approximation + cumulant correction is correct up to next-to-next-to-leading order in a systematic eikonal expansion.

However, there is no reason to limit the variational approach to high energies only since we expect it to be useful at lower energies also. Indeed, it is just one of the inherent advantages of a variational description over an expansion in some small parameter that the variational principle stretches the parameters/functions in the trial *ansatz* in such a way as to make it “optimal” even under unfavorable kinematic conditions. Unfortunately, we were not able to corroborate this expectation either by analytical or numerical methods. Obviously, a better strategy

to solve the highly nonlinear variational equations is required.

This is one of the tasks left for the future. The other one is, of course, to apply this approximation scheme to more realistic situations, *e.g.* many-body scattering. Since the case of a spherically symmetric potential $V(r)$ was only chosen to compare with a (numerically) exactly solvable model, there is no difficulty to apply our variational scheme to general potentials and scattering from few-body targets. A good step into that direction would be to compare with the Faddeev results from ref. [38] where $n + d$ scattering with a simple model potential has been evaluated numerically for energies up to 1500 MeV and compared with the Glauber approach. The path integral representation and this variational approach will certainly be also useful in attempts to evaluate the scattering amplitude by stochastic (Monte Carlo) methods [39, 40]. Finally, as the present approach relies solely on actions and not wave function(al)s rendering it *a priori* more general, it seems that applications to nonperturbative field theory may also be possible.

Appendix A. Evaluation of averages for the variational calculation

In this section, we evaluate the different averages entering the Feynman-Jensen variational principle.

We will be using a short-hand notation which simplifies the algebra considerably: first, as usual the convention that over repeated indices is summed and second that continuous variables (times) are treated the same way. More specifically, $i, j \dots = 1, 2, 3$ denote the cartesian components of vectors and matrices, $\alpha, \beta \dots = 1, 2 \dots (3 + d)$ the components of super-vectors and $A \equiv (\alpha, t)$ etc. combine discrete and continuous indices. $\mathbb{V}^T, \mathbb{I}^T \dots$ denote the transpose of the corresponding quantity. We do not distinguish between upper and lower indices. Occasionally we also use the dot to denote a scalar product between vectors or between super-vectors. Thus, for example the trial action (3.7) may be written in several different forms as

$$\begin{aligned}
 \mathcal{A}_t &\equiv \frac{m}{2} \int_{-\infty}^{+\infty} dt dt' \sum_{\alpha, \beta=1}^{3+d} \mathbb{V}_\alpha(t) \mathbb{A}_{\alpha\beta}(t, t') \mathbb{V}_\beta(t') \\
 &\quad + \int_{-\infty}^{+\infty} dt \sum_{\alpha=1}^{3+d} B_\alpha(t) \mathbb{V}_\alpha(t) \\
 &= \frac{m}{2} \mathbb{V}_\alpha(t) \mathbb{A}_{\alpha\beta}(t, t') \mathbb{V}_\beta(t') + \mathbb{B}_\alpha(t) \mathbb{V}_\alpha(t) \\
 &= \frac{m}{2} \mathbb{V}_A \mathbb{A}_{AB} \mathbb{V}_B + \mathbb{B}_A \mathbb{V}_A = \frac{m}{2} \mathbb{V}^T \mathbb{A} \mathbb{V} + \mathbb{B}^T \mathbb{V} \\
 &= \frac{m}{2} \mathbb{V} \cdot \mathbb{A} \mathbb{V} + \mathbb{B} \cdot \mathbb{V} \tag{A.1}
 \end{aligned}$$

showing the obvious advantage of a concise notation.

We first need the path integral over the trial action

$$m_0 \equiv \int \mathcal{D}^3 v \mathcal{D}^d w \exp(i\mathcal{A}_t) \tag{A.2}$$

which from the rules of Gaussian integration can be immediately computed as

$$m_0 = \frac{\text{constant}}{\text{Det}^{1/2}(\mathbb{A})} \exp\left(-\frac{i}{2m} \mathbb{B} \cdot \mathbb{A}^{-1} \mathbb{B}\right). \quad (\text{A.3})$$

Here

$$\text{Det } X = \exp[\text{Tr} \ln X] \quad (\text{A.4})$$

denotes a determinant, both in continuous (also called a functional determinant) and discrete variables and consequently “Tr” is a trace in all variables. The path integral in eq. (2.4a) is normalized such that it is unity without interaction, *i.e.* $\mathbb{B} = 0$ and $\mathbb{A} = \sigma_3$. Here σ_3 is the (extended) third Pauli matrix which appears because the kinetic term of the anti-velocity has an opposite sign, *i.e.* $\sigma_3 = \text{diag}(1, 1, 1, -1, -1, -1)$ for the “aikonal” representation which uses a 3-dimensional anti-velocity and $\sigma_3 = \text{diag}(1, 1, 1, -1)$ for the case of a 1-dimensional w . This normalization determines the constant as $\text{Det}^{1/2} \sigma_3$. Defining for convenience the vector

$$\begin{aligned} \mathbb{C} &\equiv \mathbb{A}^{-1} \mathbb{B}, \quad \text{i.e.} \quad \mathbb{C}_A = \mathbb{A}_{AB}^{-1} \mathbb{B}_B, \\ \text{or} \quad C_\alpha(t) &= \int_{-\infty}^{+\infty} dt' \mathbb{A}_{\alpha\beta}^{-1}(t, t') \mathbb{B}_\beta(t') \end{aligned} \quad (\text{A.5})$$

and using the fact that σ_3 is its own inverse we finally have

$$\begin{aligned} m_0 &= \text{Det}^{-1/2}(\sigma_3 \mathbb{A}) \exp\left(-\frac{i}{2m} \mathbb{C} \cdot \mathbb{A} \mathbb{C}\right) \\ &= \exp\left[-\frac{1}{2} \text{Tr} \ln(\sigma_3 \mathbb{A}) - \frac{i}{2m} \mathbb{C} \cdot \mathbb{A} \mathbb{C}\right]. \end{aligned} \quad (\text{A.6})$$

This will also serve as a master integral or generating function for the averages we have to calculate.

The Feynman-Jensen variational principle requires the average of the difference between the full action and the trial action

$$\langle \Delta \mathcal{A} \rangle_t = \frac{m}{2} \langle \mathbb{V} \cdot (\sigma_3 - \mathbb{A}) \mathbb{V} \rangle_t - \langle \mathbb{B} \cdot \mathbb{V} \rangle_t + \langle \chi \rangle_t. \quad (\text{A.7})$$

Here

$$\chi(\mathbf{b}, \mathbb{V}) = - \int_{-\infty}^{+\infty} dt V(\mathbf{x}_{\text{ref}}(t) + \mathbf{x}_{\text{quant}}(t)) \quad (\text{A.8})$$

is the phase in the path integral (2.4a) for the impact-parameter \mathcal{S} -matrix and the average has been defined in eq. (3.4).

Appendix A.1. Computation of $\langle \mathbb{B} \cdot \mathbb{V} \rangle_t$

The evaluation of this average is easily done by putting an artificial scalar factor a in the linear term of the trial

action and differentiating with respect to this factor

$$\begin{aligned} \langle \mathbb{B} \cdot \mathbb{V} \rangle_t &= -i \frac{d}{da} \ln m_0(\mathbb{C} \rightarrow a\mathbb{C}) \Big|_{a=1} \\ &= -i \frac{d}{da} \left(-i \frac{a^2}{2m} \mathbb{C} \cdot \mathbb{A} \mathbb{C} \right) \Big|_{a=1} \\ &= -\frac{1}{m} \mathbb{C} \cdot \mathbb{A} \mathbb{C}. \end{aligned} \quad (\text{A.9})$$

Appendix A.2. Computation of $\frac{m}{2} \langle \mathbb{V} \cdot (\sigma_3 - \mathbb{A}) \mathbb{V} \rangle_t$

We obtain this average by the same technique: differentiating m_0 with respect to \mathbb{B} brings down a factor \mathbb{V} . Therefore

$$\begin{aligned} \frac{m}{2} \langle \mathbb{V} \cdot (\sigma_3 - \mathbb{A}) \mathbb{V} \rangle_t &= -\frac{1}{m_0} \frac{m}{2} \frac{\delta^2 m_0}{\delta \mathbb{B}_\beta(t') \delta \mathbb{B}_\alpha(t)} \\ &\times \left[\sigma_3^{\alpha\beta} \delta(t-t') - \mathbb{A}^{\alpha\beta}(t, t') \right]. \end{aligned} \quad (\text{A.10})$$

After the insertion of

$$\frac{\delta^2 m_0}{\delta \mathbb{B}_\beta(t') \delta \mathbb{B}_\alpha(t)} = m_0 \left[-\frac{1}{m^2} \mathbb{C}_\alpha(t) \mathbb{C}_\beta(t') - \frac{i}{m} \mathbb{A}_{\alpha\beta}^{-1}(t, t') \right] \quad (\text{A.11})$$

we obtain

$$\begin{aligned} \frac{m}{2} \langle \mathbb{V} \cdot (\sigma_3 - \mathbb{A}) \mathbb{V} \rangle_t &= -\frac{m}{2} \left[-\frac{1}{m^2} \mathbb{C}_A(t) \mathbb{C}_B(t') \right. \\ &\left. - \frac{1}{m} \mathbb{A}_{AB}^{-1}(t, t') \right] \left[\sigma_3^{AB}(t, t') - \mathbb{A}^{AB}(t, t') \right], \end{aligned} \quad (\text{A.12})$$

or, in continuous notation,

$$\begin{aligned} \frac{m}{2} \langle \mathbb{V} \cdot (\sigma_3 - \mathbb{A}) \mathbb{V} \rangle_t &= \frac{1}{2m} [\mathbb{C} \cdot \sigma_3 \mathbb{C} - \mathbb{C} \cdot \mathbb{A} \mathbb{C}] \\ &+ \frac{i}{2} \text{Tr} [\sigma_3 \mathbb{A}^{-1} - 1]. \end{aligned} \quad (\text{A.13})$$

Together with eqs. (A.6) and (A.9) we thus have for the variational functional

$$\begin{aligned} S(\mathbf{b}, \mathbb{A}, \mathbb{C}) &= \exp \left\{ \frac{i}{2m} \mathbb{C} \cdot \sigma_3 \mathbb{C} - \frac{1}{2} \text{Tr} [\ln(\sigma_3 \mathbb{A}) \right. \\ &\left. + \sigma_3 \mathbb{A}^{-1} - 1] + i \langle \chi \rangle_t \right\}. \end{aligned} \quad (\text{A.14})$$

Appendix A.3. Computation of $\langle \chi \rangle_t$

Finally the average over the phase (A.8) can be done by a Fourier transformation of the potential:

$$\begin{aligned} \langle \chi \rangle_t &= - \int_{-\infty}^{+\infty} dt \int \frac{d^3 p}{(2\pi)^3} \tilde{V}(\mathbf{p}) \exp[i\mathbf{p} \cdot \mathbf{x}_{\text{ref}}(t)] \\ &\times \langle \exp(i\mathbf{p} \cdot \mathbf{x}_{\text{quant}}(t)) \rangle_t. \end{aligned} \quad (\text{A.15})$$

$$\Gamma(t, t') = \frac{1}{2} \begin{pmatrix} \text{sgn}(t-t') & 0 & 0 & -\text{sgn}(-t') & 0 & 0 \\ 0 & \text{sgn}(t-t') & 0 & 0 & -\text{sgn}(-t') & 0 \\ 0 & 0 & \text{sgn}(t-t') & 0 & 0 & -\text{sgn}(-t') \end{pmatrix}, \quad (\text{A.17})$$

$$\Gamma(t, t') = \frac{1}{2} \begin{pmatrix} \text{sgn}(t-t') - \text{sgn}(-t') & 0 & 0 & 0 \\ 0 & \text{sgn}(t-t') - \text{sgn}(-t') & 0 & 0 \\ 0 & 0 & \text{sgn}(t-t') - \text{sgn}(-t') & 0 \end{pmatrix}, \quad (\text{A.18})$$

To simplify the calculation we write

$$\begin{aligned} \mathbf{x}_{\text{quant}}(t) &=: \Gamma(t, t') \nabla(t'), \\ \text{i.e. } x_{\text{quant}}^i(t) &= \int_{-\infty}^{+\infty} dt' \Gamma_{i\alpha}(t, t') \nabla_{\alpha}(t'), \end{aligned} \quad (\text{A.16})$$

where $\Gamma_{i\beta}(t, t')$ is a $3 \times (3+d)$ -matrix operator. Note that as a messenger between ordinary space and the “super”-space in which velocity + anti-velocity live it cannot be a square matrix. Indeed, from the connection (2.6) between quantum fluctuation and velocity we immediately find

see eq. (A.17) on top of the page

for the “aikonal” case and from eq. (2.9)

see eq. (A.18) on top of the page

for the “ray” case if we choose the mean momentum along the 3-axis.

In any case the average in eq. (A.15) involves only Gaussian integrals where in the exponent the

$$\begin{aligned} \text{term linear in } \mathbb{V} &= \\ \begin{cases} i [\mathbb{B}_{\alpha} + p_i \Gamma_{i\alpha}] \mathbb{V}_{\alpha} & \text{for the numerator,} \\ i \mathbb{B} \cdot \mathbb{V} & \text{for the denominator.} \end{cases} \end{aligned} \quad (\text{A.19})$$

Thus,

$$\begin{aligned} &\langle \exp(i \mathbf{p} \cdot \mathbf{x}_{\text{quant}}(t)) \rangle_t \\ &= \frac{1}{m_0} \int \mathcal{D}^3 \mathcal{D}^d w \exp \left\{ i \frac{m}{2} \mathbb{V}^T \mathbb{A} \mathbb{V} + i [\mathbb{B} + \mathbf{p} \cdot \Gamma(t, \cdot)] \cdot \mathbb{V} \right\} \\ &= \exp \left\{ - \frac{i}{2m} [\mathbb{B}_{\alpha}(t') + p_i \Gamma_{i\alpha}(t, t')] \mathbb{A}_{\alpha\beta}^{-1}(t', t'') \right. \\ &\quad \left. \times [\mathbb{B}_{\beta}(t'') + p_j \Gamma_{j\beta}(t, t'')] \right\} \\ &\quad \times \exp \left\{ \frac{i}{2m} \mathbb{B} \cdot \mathbb{A}^{-1} \mathbb{B} \right\}, \end{aligned} \quad (\text{A.20})$$

where the last factor comes from the normalization of the average by $1/m_0$ and no summation/integration over the external time-parameter t is implied. Working out the exponential we find terms linear and quadratic in \mathbf{p} while the constant term cancels. The term linear in \mathbf{p} gives the trajectory

$$\boldsymbol{\rho}_i(t) := \mathbf{x}_{\text{ref}}^i(t) - \frac{1}{m} \Gamma_{i\alpha}(t, t') \mathbb{A}_{\alpha\beta}^{-1}(t', t'') \mathbb{B}_{\beta}(t''), \quad (\text{A.21})$$

or in short-hand notation

$$\boldsymbol{\rho}(t) = \mathbf{x}_{\text{ref}}(t) - \frac{1}{m} \Gamma(t, \cdot) \mathbb{C}. \quad (\text{A.22})$$

The term quadratic in \mathbf{p} reads

$$-\frac{i}{2m} p_i \Gamma_{i\alpha}(t, t') \mathbb{A}_{\alpha\beta}^{-1}(t', t'') \Gamma_{j\beta}(t, t'') p_j \quad (\text{A.23})$$

which becomes $-(1/2)p_i p_j \sigma_{ij}(t)$ if a square (3×3) -matrix

$$\begin{aligned} \sigma_{ij}(t) &= \frac{i}{m} \Gamma_{i\alpha}(t, t') \Gamma_{j\beta}(t, t'') \mathbb{A}_{\alpha\beta}^{-1}(t', t''), \\ \text{or } \sigma(t) &= \frac{i}{m} \Gamma(t, \cdot) \mathbb{A}^{-1} \Gamma^T(\cdot, t) \end{aligned} \quad (\text{A.24})$$

is defined (again no summation/integration over the external t). From the definition (3.14) for the Gaussian transform of the potential we then obtain the following simple expression for $\langle \chi \rangle_t$:

$$\langle \chi \rangle_t = - \int_{-\infty}^{+\infty} dt V_{\sigma(t)}(\boldsymbol{\rho}(t)). \quad (\text{A.25})$$

Appendix B. Variational equations

In appendix A we have calculated the quantities to be varied in the Feynman-Jensen functional. The result (A.14) may be written as

$$S(\mathbf{b}, \mathbb{A}, \mathbb{C}) = \exp [iX_0 + iX_1 - \Omega(\sigma_3 \mathbb{A})], \quad (\text{B.1})$$

with

$$X_0 \equiv \langle \chi \rangle_t = - \int_{-\infty}^{+\infty} dt V_{\sigma(t)}(\boldsymbol{\rho}(t)), \quad (\text{B.2})$$

$$X_1 := \frac{1}{2m} \mathbb{C} \cdot \sigma_3 \mathbb{C}, \quad (\text{B.3})$$

$$\Omega(X) := \frac{1}{2} \text{Tr} [\ln X + X^{-1} - 1]. \quad (\text{B.4})$$

The argument of the potential—the trajectory—is given in eq. (A.22) and its Gaussian width in eq. (A.24). We will now compute the variational equations for \mathbb{A} and \mathbb{B} which follow when stationarity of $S(\mathbf{b}, \mathbb{A}, \mathbb{B})$ is required. However, since only the combination $\mathbb{C} = \mathbb{A}^{-1} \mathbb{B}$ (but not \mathbb{B}) and \mathbb{A}^{-1} enter the functional to be varied, it is more convenient to vary with respect to \mathbb{C} and \mathbb{A}^{-1} .

Appendix B.1. Variational equation for \mathbb{C}

The vector \mathbb{C} only shows up in the phase X_1 and the trajectory $\boldsymbol{\rho}(t)$. Therefore stationarity of the variational functional requires

$$\frac{\delta X_1}{\delta \mathbb{C}_\alpha(t)} - \int_{-\infty}^{+\infty} dt' \partial_i V_{\sigma(t')}(\boldsymbol{\rho}(t')) \frac{\delta \boldsymbol{\rho}_i(t')}{\delta \mathbb{C}_\alpha(t)} \stackrel{!}{=} 0, \quad (\text{B.5})$$

where we have used the chain rule in the last term. From eq. (B.3) we immediately have

$$\frac{\delta X_1}{\delta \mathbb{C}_\alpha(t)} = \frac{1}{m} (\sigma_3 \mathbb{C})_\alpha(t) \quad (\text{B.6})$$

and from eq. (A.22)

$$\frac{\delta \boldsymbol{\rho}_i(t')}{\delta \mathbb{C}_\alpha(t)} = -\frac{1}{m} \Gamma_{i\alpha}(t', t). \quad (\text{B.7})$$

Thus,

$$(\sigma_3 \mathbb{C})_\alpha(t) = -\partial_i V_\sigma(t') \Gamma_{i\alpha}(t', t). \quad (\text{B.8})$$

As σ_3 is its own inverse and diagonal in the time variables, we may solve this as

$$\mathbb{C}_\alpha(t) = -(\sigma_3)_{\alpha\beta} \partial_i V_\sigma(t') \Gamma_{i\beta}(t', t), \quad (\text{B.9})$$

or

$$\mathbb{C}_{\text{var}} = -\sigma_3 \Gamma^T \mathbf{J}_\sigma, \quad (\text{B.10})$$

where

$$\mathbf{J}_\sigma(t) = \nabla V_{\sigma(t)}(\boldsymbol{\rho}(t)) \quad (\text{B.11})$$

is the vector of potential derivatives (also called the Jacobian). We can now put this expression into the trajectory to get

$$\begin{aligned} \boldsymbol{\rho}_{\text{var}}(t) &= \mathbf{x}_{\text{ref}}(t) - \frac{1}{m} \Gamma(t, s) \mathbb{C}^{\text{var}}(s) \\ &= \mathbf{x}_{\text{ref}}(t) + \frac{1}{m} \Gamma(t, s) \sigma_3 \Gamma^T(s, t') \mathbf{J}_\sigma(t') \\ &=: \mathbf{x}_{\text{ref}}(t) + \Sigma_0(t, t') \mathbf{J}_\sigma(t'). \end{aligned} \quad (\text{B.12})$$

$$\Sigma_0(t, t') := \frac{1}{m} \Gamma(t, s) \sigma_3 \Gamma^T(s, t'), \quad (\text{B.13})$$

Here we have defined the (3×3) -matrix

$$\Sigma_0(t, t') := \frac{1}{m} \Gamma(t, s) \sigma_3 \Gamma^T(s, t'), \quad (\text{B.14})$$

whose explicit form can be worked out with the help of eqs. (A.17) and (A.18) and the relation

$$\int_{-T}^{+T} ds \operatorname{sgn}(s-t) \operatorname{sgn}(s-t') = 2[T - |t-t'|]. \quad (\text{B.15})$$

Due to the contribution from the anti-velocity all terms which would diverge for $T \rightarrow \infty$ cancel and one obtains the expressions given in eqs. (3.18) and (3.19a). Note that Σ_0 is the Green function for the corresponding equation of motion. For example, we have

$$-m \frac{\partial^2}{\partial t^2} \left(\Sigma_0^{(3-3)} \right)_{ij}(t, t') = \delta(t-t') \delta_{ij}, \quad (\text{B.16})$$

so that one can write

$$\Sigma_0^{(3-3)} = \mathcal{P} \frac{1}{-m \partial_t^2}, \quad (\text{B.17})$$

where \mathcal{P} denotes the principal value prescription. Indeed, evaluating in Fourier (E -) space with $\langle E|t \rangle = \exp(iEt)/\sqrt{2\pi}$ as transformation function we obtain

$$\begin{aligned} \left(\Sigma_0^{(3-3)} \right)_{ij}(t, t') &= \frac{\delta_{ij}}{m} \frac{1}{2\pi} \mathcal{P} \int_{-\infty}^{+\infty} dE \frac{\exp(iE(t-t'))}{E^2} \\ &\equiv \frac{\delta_{ij}}{m} \frac{1}{2\pi} \int_{-\infty}^{+\infty} dE \frac{\exp(iE(t-t')) - 1}{E^2} \\ &= -\frac{\delta_{ij}}{m} \frac{1}{\pi} \int_0^\infty dE \frac{1 - \cos(E(t-t'))}{E^2} = -\frac{1}{2m} |t-t'| \delta_{ij}, \end{aligned} \quad (\text{B.18})$$

in agreement with eq. (3.18).

Appendix B.2. Variational equation for \mathbb{A}^{-1}

The matrix \mathbb{A}^{-1} only enters in the Gaussian width σ (appearing in X_0) and in the ‘‘fluctuation term’’ Ω . Therefore requiring stationarity means

$$-\frac{\delta \Omega}{\delta \mathbb{A}_{\alpha\beta}^{-1}(t_1, t_2)} - i \int_{-\infty}^{+\infty} dt \frac{\delta V_\sigma(t)}{\delta \mathbb{A}_{\alpha\beta}^{-1}(t_1, t_2)} \stackrel{!}{=} 0. \quad (\text{B.19})$$

From the definition (3.14) we find

$$\frac{\delta V_\sigma(t)}{\delta \mathbb{A}_{\alpha\beta}^{-1}(t_1, t_2)} = \frac{1}{2} \partial_i \partial_j V_\sigma(t) \frac{\delta \sigma_{ij}(t)}{\delta \mathbb{A}_{\alpha\beta}^{-1}(t_1, t_2)}. \quad (\text{B.20})$$

Thus, we have to compute the functional derivative of the Gaussian width and fluctuation term with respect to \mathbb{A}^{-1} . This is easily done for the Gaussian width: from eq. (A.24) it follows:

$$\frac{\delta \sigma_{ij}(t)}{\delta \mathbb{A}_{\alpha\beta}^{-1}(t_1, t_2)} = \frac{i}{m} \Gamma_{i\alpha}(t, t_1) \Gamma_{j\beta}(t, t_2). \quad (\text{B.21})$$

For the fluctuation term we rewrite eq. (B.4) as

$$\Omega(\sigma_3 \mathbb{A}) = \frac{1}{2} \operatorname{Tr} [-\ln(\mathbb{A}^{-1} \sigma_3) + (\mathbb{A}^{-1} \sigma_3) - 1] \quad (\text{B.22})$$

and use the chain rule (in our condensed notation from appendix A)

$$\begin{aligned} \frac{\partial \Omega(\mathbb{A}^{-1} \sigma_3)}{\partial \mathbb{A}_{AB}^{-1}} &= \frac{\partial \Omega(\mathbb{A}^{-1} \sigma_3)}{\partial [\mathbb{A}^{-1} \sigma_3]_{CD}} \frac{[\partial \mathbb{A}^{-1} \sigma_3]_{CD}}{\partial \mathbb{A}_{AB}^{-1}} \\ &= \frac{\partial \Omega(\mathbb{A}^{-1} \sigma_3)}{\partial [\mathbb{A}^{-1} \sigma_3]_{CD}} \delta_{AC}(\sigma_3)_{BD}. \end{aligned} \quad (\text{B.23})$$

Since⁸

$$\frac{\partial \operatorname{Tr} f(X)}{\partial X_{CD}} = [f'(X)]_{DC} \quad (\text{B.24})$$

⁸ This can be easily proved by a power series expansion of $f(X)$, piecewise differentiation and resumming.

for any differentiable function $f(X)$ we obtain

$$\begin{aligned} \frac{\partial \Omega(\mathbb{A}^{-1}\sigma_3)}{\partial \mathbb{A}_{AB}^{-1}} &= -\frac{1}{2} \left\{ \left([\mathbb{A}^{-1}\sigma_3]^{-1} \right)_{DC} - \delta_{AD} \right\} \delta_{AC} (\sigma_3)_{BD} \\ &= -\frac{1}{2} \{ \mathbb{A}_{AB} - [\sigma_3]_{AB} \}, \end{aligned} \quad (\text{B.25})$$

where we used the fact both σ_3 and \mathbb{A} are symmetric. In extended notation the results reads

$$\frac{\delta \Omega(\sigma_3 \mathbb{A})}{\delta \mathbb{A}_{\alpha\beta}^{-1}(t_1, t_2)} = -\frac{1}{2} \{ \mathbb{A}_{\alpha\beta}(t_1, t_2) - (\sigma_3)_{\alpha\beta} \delta(t_1 - t_2) \}. \quad (\text{B.26})$$

Utilizing eqs. (B.20), (B.21) the variational equation (B.19) therefore becomes

$$\begin{aligned} -\frac{1}{2} \{ \mathbb{A}_{\alpha\beta}(t_1, t_2) - (\sigma_3)_{\alpha\beta} \delta(t_1 - t_2) \} = \\ \frac{1}{2m} \int_{-\infty}^{+\infty} dt \partial_i \partial_j V_\sigma(t) \Gamma_{i\alpha}(t, t_1) \Gamma_{j\beta}(t, t_2). \end{aligned} \quad (\text{B.27})$$

In matrix notation this simply reads

$$\mathbb{A}_{\text{var}} = \sigma_3 - \frac{1}{m} \Gamma^T H_\sigma \Gamma \quad (\text{B.28})$$

where H_σ stands for the matrix of second derivatives (also called the Hessian) of the potential

$$H_\sigma^{ij}(t, t') := \partial_i \partial_j V_{\sigma(t)}(\boldsymbol{\rho}(t)) \delta(t - t'). \quad (\text{B.29})$$

It is possible to put the results in an even more compact form by defining

$$\Sigma := \frac{1}{m} \Gamma \mathbb{A}^{-1} \Gamma^T. \quad (\text{B.30})$$

Note that for the free case $\mathbb{A} = \sigma_3$ this reduces to the matrix Σ_0 defined in eq. (B.14) which is the Green function for the equation of motion (B.13). Multiplying eq. (B.28) from left by $\Gamma \sigma_3$ and from right by $\mathbb{A}^{-1} \Gamma^T / m$, the variational equation for \mathbb{A}^{-1} then translates into a Lippmann-Schwinger-like integral equation

$$\Sigma = \Sigma_0 + \Sigma_0 H_\sigma \Sigma. \quad (\text{B.31})$$

All relevant quantities can be written in terms of $\Sigma(t, t')$ and the variational trajectory $\boldsymbol{\rho}(t)$. For instance from eqs. (B.3), (B.10) and (B.14) we immediately obtain

$$X_1 = \frac{1}{2} \mathbf{J}_\sigma \cdot \Sigma_0 \mathbf{J}_\sigma. \quad (\text{B.32})$$

Less obvious is that the fluctuation term $\Omega(\sigma_3 \mathbb{A})$ defined in eq. (B.4) may also be expressed in terms of Σ and $\boldsymbol{\rho}$. However, if the variational solution (B.28) is multiplied by \mathbb{A}^{-1} and inserted into

$$\Omega(\sigma_3 \mathbb{A}) = -\frac{1}{2} \text{Tr} [\ln(\mathbb{A}^{-1} \sigma_3) - \mathbb{A}^{-1} \sigma_3 + 1] \quad (\text{B.33})$$

one obtains

$$\Omega_{\text{var}} = -\frac{1}{2} \text{Tr} \left[\ln \left(1 + \mathbb{A}^{-1} \frac{1}{m} \Gamma^T H_\sigma \Gamma \right) - \frac{1}{m} \mathbb{A}^{-1} \Gamma^T H_\sigma \Gamma \right]. \quad (\text{B.34})$$

Using the definition (B.30) and the properties of the trace this becomes

$$\Omega = -\frac{1}{2} \text{Tr} [\ln(1 + \Sigma H_\sigma) - \Sigma H_\sigma]. \quad (\text{B.35})$$

Finally, from eq. (A.24) we see that the Gaussian width $\sigma(t)$ is just given by the diagonal element of $i\Sigma$.

Appendix C. Calculation of the second cumulant

In this section we compute the first correction to the variational approximation, *i.e.* the second cumulant

$$\lambda_2 = \langle (\Delta \mathcal{A})^2 \rangle_t - \langle \Delta \mathcal{A} \rangle_t^2, \quad (\text{C.1})$$

$$\Delta \mathcal{A} = \frac{m}{2} \mathbb{V} \cdot (\sigma_3 - \mathbb{A}) \mathbb{V} - \mathbb{B} \cdot \mathbb{V} + \chi, \quad (\text{C.2})$$

for both representations. Since the computational steps are similar to the ones in appendix A we will not enter into too much details. After some algebra we find that the second cumulant is given by the following terms which we will evaluate subsequently:

$$\begin{aligned} \lambda_2 &= \langle \chi^2 \rangle_t - \langle \chi \rangle_t^2 + \frac{i}{m} \mathbf{C} \cdot \mathbb{A} \mathbf{C} + im \left. \frac{d}{da} \right|_{a=1} \\ &\times \left[\langle E_a \rangle_t + \frac{2}{m} \langle \chi_a \rangle_t \right] - [(\sigma_3)_{\alpha\beta}(t, t') - \mathbb{A}_{\alpha\beta}(t, t')] \\ &\times \left[2 \frac{m}{m_0} \frac{\delta m_0}{\delta \mathbb{B}_\alpha(t)} \frac{\delta \langle \chi \rangle_t}{\delta \mathbb{B}_\beta(t')} + m \frac{\delta^2 \langle \chi \rangle_t}{\delta \mathbb{B}_\alpha(t) \delta \mathbb{B}_\beta(t')} \right. \\ &\left. + \frac{m^2}{2m_0} \frac{\delta m_0}{\delta \mathbb{B}_\alpha(t)} \frac{\delta \langle E \rangle_t}{\delta \mathbb{B}_\beta(t')} + \frac{m^2}{4} \frac{\delta^2 \langle E \rangle_t}{\delta \mathbb{B}_\alpha(t) \delta \mathbb{B}_\beta(t')} \right], \end{aligned} \quad (\text{C.3})$$

where the quantity E stands for

$$\langle E \rangle_t := \langle \mathbb{V} \cdot (\sigma_3 - \mathbb{A}) \mathbb{V} \rangle_t. \quad (\text{C.4})$$

From our study of the first cumulant, eqs. (A.13) and (A.25), we can compute

$$\left. \frac{d}{da} \right|_{a=1} \langle \chi_a \rangle_t = \frac{1}{m} \nabla V_\sigma \cdot \Gamma \mathbf{C}, \quad (\text{C.5})$$

and

$$\left. \frac{d}{da} \right|_{a=1} \langle E_a \rangle_t = \frac{2}{m^2} [\mathbf{C} \cdot \sigma_3 \mathbf{C} - \mathbf{C} \cdot \mathbb{A} \mathbf{C}]. \quad (\text{C.6})$$

Similarly, we have

$$\frac{1}{m_0} \frac{\delta m_0}{\delta \mathbb{B}_\alpha(t)} = -\frac{i}{m} \mathbf{C}_\alpha(t), \quad (\text{C.7})$$

$$\frac{\delta \langle \chi \rangle_t}{\delta \mathbb{B}_\alpha(t)} = \frac{1}{m} [\nabla V_\sigma \cdot \Gamma \mathbb{A}^{-1}]_\alpha(t), \quad (\text{C.8})$$

$$\frac{\delta \langle E \rangle_t}{\delta \mathbb{B}_\alpha(t)} = \frac{2}{m^2} [\mathbf{C} \cdot \sigma_3 \mathbb{A}^{-1} - \mathbf{C}]_\alpha(t), \quad (\text{C.9})$$

while

$$\frac{\delta^2 \langle E \rangle_t}{\delta \mathbb{B}_\alpha(t) \delta \mathbb{B}_\beta(t')} = \frac{2}{m^2} [\mathbb{A}^{-1} \sigma_3 \mathbb{A}^{-1} - \mathbb{A}^{-1}]_{\alpha\beta}(t, t'), \quad (\text{C.10})$$

$$\frac{\delta^2 \langle \chi \rangle_t}{\delta \mathbb{B}_\alpha(t) \delta \mathbb{B}_\beta(t')} = -\frac{1}{m^2} [\mathbb{A}^{-1} \Gamma^T H_\sigma \Gamma \mathbb{A}^{-1}]_{\alpha\beta}(t, t') \quad (\text{C.11})$$

$$\stackrel{\text{var}}{=} -\frac{1}{m} [\mathbb{A}^{-1} (\sigma_3 - \mathbb{A}) \mathbb{A}^{-1}]_{\alpha\beta}(t, t'). \quad (\text{C.12})$$

Here, the “var” above the equality sign in the last line means that the variational solution (B.28) has been used. We have now everything needed to compute the second cumulant. After some (tedious) algebra we obtain

$$\lambda_2 = \langle \chi^2 \rangle_t - \langle \chi \rangle_t^2 - \frac{i}{m} \mathbb{C} \cdot \sigma_3 \mathbb{A}^{-1} \sigma_3 \mathbb{C} + \frac{1}{2} \times \text{Tr} [\mathbb{A}^{-1} \sigma_3 \mathbb{A}^{-1} \sigma_3 - 1] - \text{Tr} [\mathbb{A}^{-1} \sigma_3 - 1]. \quad (\text{C.13})$$

Using the variational equations and the Lippmann-Schwinger-like equation we find

$$\text{Tr} [\sigma_3 \mathbb{A}^{-1} - 1] = \text{Tr} [\Sigma H_\sigma], \quad (\text{C.14})$$

$$\frac{1}{2} \text{Tr} [\sigma_3 \mathbb{A}^{-1} \sigma_3 \mathbb{A}^{-1} - 1] = \text{Tr} \left[\Sigma H_\sigma + \frac{1}{2} (\Sigma H_\sigma)^2 \right], \quad (\text{C.15})$$

while

$$\frac{i}{m} \mathbb{C} \cdot \sigma_3 \mathbb{A}^{-1} \sigma_3 \mathbb{C} = i \nabla V_\sigma^T \Sigma \nabla V_\sigma, \quad (\text{C.16})$$

so that our final result is

$$\lambda_2 = \langle \chi^2 \rangle_t - \langle \chi \rangle_t^2 - i \nabla V_\sigma^T \Sigma \nabla V_\sigma + \frac{1}{2} \text{Tr} [\Sigma H_\sigma]^2. \quad (\text{C.17})$$

The quantity $\langle \chi^2 \rangle_t$ is evaluated in the very same way as $\langle \chi \rangle_t$, *i.e.* one transforms the potential to Fourier space, and performs the functional integrations. The result is the one given in eq. (3.27).

Appendix D. Some numerical details

Here we discuss several points which are essential to obtain reliable numerical values for our variational approximations.

Appendix D.1. Variables

As the range of the potential greatly determines the dynamics of the scattering process we switch from time variables to distances by substituting

$$t = \frac{z}{v_{\text{char}}}, \quad (\text{D.1})$$

where the characteristic velocity is chosen as the asymptotic velocity on the different reference trajectories, *viz.*

$$v_{\text{char}} = \begin{cases} \frac{K}{m}: & \text{“aikonal”}, \\ \frac{k}{m}: & \text{“ray”}. \end{cases} \quad (\text{D.2})$$

This is reasonable for high-energy scattering where indeed the particle mostly travels along the reference trajectory and implies that each power of t and each integration over t is suppressed by an inverse power of K (or k). It becomes less convincing at low energy where the characteristic velocity may be totally different from the asymptotic one—for example, in scattering via a resonance. However, all our applications will be in the high-energy domain.

Appendix D.2. Numerical integration

Initially, our numerical integrations have been performed by using Gauss-Legendre quadrature rules for a *finite* interval $[-z_{\text{max}}, +z_{\text{max}}]$. Typically, we have taken

$$z_{\text{max}} \sim (4-6) \cdot R \quad (\text{D.3})$$

as we expect that outside this interval the potential is practically zero. Of course, z_{max} had to be varied to ensure stable results. In previous work we had mapped the *infinite* z -interval to a finite one (for example by $z = R \tan \psi$) but in the present case this caused some problems for the iterative solution of the variational equations which are avoided if the integration is over a finite, not too large interval.

The numerical integration was performed with n_e subdivisions and n_g Gaussian points in each subinterval requiring $N = n_e \times n_g$ function calls altogether. Again the number n_e was varied to verify stability of the results whereas the number n_g was kept fixed at moderate values which is advisable for oscillatory integrands, *e.g.* $(n_g, n_e) = (32, 2)$. Since we deal with multi-dimensional integrals and have to solve the variational equations for each \mathbf{b} -value on the grid the computing time rapidly increases when making the grid finer and finer and at large scattering angles (where the scattering amplitude becomes small by interference) it became difficult to obtain stable numerical results. In these cases use of the adaptive routine DCUHRE [41, 42] for the \mathbf{b} -integration was quite helpful as it chooses the integration points according to their relative importance.

Later we realized that integrating numerically over nonanalytic functions like $|z-z'|$ or $|z'|$ (which occur in the Green function $\Sigma_0(z, z')$) is not well handled by Gaussian or similar quadrature rules. The reason is that their error is proportional to some high derivative of the integrand within the integration interval which makes them suitable for analytic functions but not for nonanalytic ones. Consequently, the simple trapezoidal rule (see, *e.g.* eq. (25.4.2) in ref. [43], with $h = (z_N - z_0)/N$ denoting the increment)

$$\int_{z_0}^{z_N} dz f(z) = h \left[\frac{f_0}{2} + f_1 + \dots + f_{N-1} + \frac{f_N}{2} \right] - \frac{N h^3}{12} f''(\xi), \quad z_0 < \xi < z_N \quad (\text{D.4})$$

Table 4. Maximal deviation of the numerically evaluated integrals $I_{1/2}(z)$ (see eqs. (D.5), (D.6)) from the exact value for different quadrature rules and function calls N in the interval $z \in [-5, 5]$. The integration range was made finite by cutting off the integrand for $|z'| > 5$. “Gauss 24” etc. refers to a Gauss-Legendre quadrature rule with $n_g = 24$ points etc. The last two lines give the results obtained with the Euler-MacLaurin summation formula retaining corrections up to second and fourth power in the increment, respectively, due to the nonanalytic behaviour of the integrand.

Rule	$I_1(z)$				$I_2(z)$			
	N				N			
	24	48	72	144	24	48	72	144
Gauss 24	6.38 (-2)	5.12 (-3)	7.53 (-3)	1.24 (-3)	1.01 (-1)	5.12 (-3)	1.14 (-2)	1.24 (-3)
Gauss 48		1.72 (-2)		1.94 (-3)		2.61 (-2)		2.91 (-3)
Gauss 72			7.77 (-3)	5.80 (-4)			1.17 (-2)	5.78 (-4)
Simpson	5.04 (-2)	1.40 (-2)	6.34 (-3)	1.60 (-3)	5.30 (-2)	1.42 (-2)	6.37 (-3)	1.60 (-3)
Trapez	2.95 (-2)	7.27 (-3)	3.22 (-3)	8.04 (-4)	-2.95 (-2)	-7.27 (-3)	-3.22 (-3)	-8.04 (-4)
Euler-MacLaurin ₂	5.25 (-4)	3.17 (-5)	6.23 (-6)	3.88 (-7)	-7.57 (-4)	-4.59 (-5)	-9.01 (-6)	-5.61 (-7)
Euler-MacLaurin ₄	6.33 (-5)	1.00 (-6)	8.81 (-8)	1.39 (-9)	-9.91 (-5)	-1.60 (-6)	-1.43 (-7)	-2.23 (-9)

is as efficient (or better: inefficient) in integrating nonanalytic functions as a N -point Gaussian integration which is exact for polynomials up to z^{2N-1} or Simpson’s rule whose error is proportional to $h^5 f^{(4)}(\xi)$. This is demonstrated in table 4 where the test cases

$$I_1(z) := \int_{-\infty}^{+\infty} dz' |z - z'| e^{-z'^2} = \sqrt{\pi} z \cdot \operatorname{erf}(z) + e^{-z^2}, \quad (\text{D.5})$$

$$I_2(x) := \int_{-\infty}^{+\infty} dz' \left\{ |z - z'| - |z| - |z'| \right\} e^{-z'^2} \\ = I_1(z) - \sqrt{\pi} |z| - 1, \quad (\text{D.6})$$

are considered as typical examples of integrals for a Gaussian potential in the “aikonal” and the “ray” representation, respectively. Here $\operatorname{erf}(z)$ denotes the standard error function with $\operatorname{erf}(-z) = -\operatorname{erf}(z)$. It is obvious that the accuracy is relatively poor and the convergence with increasing number N of function calls is disappointingly slow⁹. This can be improved in the following way:

For simplicity, we first consider integrands of the I_1 -type, *i.e.*

$$f(z') = |z - z'| \phi(z') + g(z'), \quad (\text{D.7})$$

where $\phi(z')$, $g(z')$ are differentiable functions which vanish rapidly enough for $z' \rightarrow \pm\infty$. Therefore to a good approximation

$$\int_{-\infty}^{+\infty} dz' \left\{ |z - z'| \phi(z') + g(z') \right\} \simeq \\ \int_{-z_{\max}}^z dz' \left[(z - z') \phi(z') + g(z') \right] \\ + \int_z^{+z_{\max}} dz' \left[(z' - z) \phi(z') + g(z') \right]. \quad (\text{D.8})$$

⁹ For comparison: without absolute sign in the integrand, *i.e.* for an analytic function, the absolute deviation from the exact result is lower than 10^{-11} already at $N = 48$ for all integration rules. Strictly speaking, of course, the equally spaced rules require $N + 1$ function calls.

Note that the integrand is analytic but different in the two integrals. We may now apply the Euler-MacLaurin summation formula (ref. [43], eq. (25.4.7)) assuming that the point of nonanalyticity $z = kh$ is a multiple of the increment $h = 2z_{\max}/N$. As we are evaluating the variational equations iteratively on a grid this certainly is the case and we obtain

$$\int_{-z_{\max}}^{+z_{\max}} dz' \left\{ |z - z'| \phi(z') + g(z') \right\} \simeq \text{trapezoidal rule} \\ - \sum_{m=1}^n \frac{B_{2m} h^{2m}}{(2m)!} \left\{ \frac{d^{2m-1}}{dz'^{2m-1}} [(z - z') \phi(z') + g(z')] \right. \\ \left. - \frac{d^{2m-1}}{dz'^{2m-1}} [(z' - z) \phi(z') + g(z')] \right\}_{z'=z} = \\ \text{trapezoidal rule} + \frac{h^2}{6} \phi_k - \frac{h^4}{120} \phi_k'' + \mathcal{O}(h^6). \quad (\text{D.9})$$

where B_{2m} are the Bernoulli numbers. Note that the correction terms come from discontinuities of derivatives of the integrands below and above the point $z = kh$ (we neglect the contributions around the endpoints at $\pm z_{\max}$ since the integrand is assumed to be very small there). The integration rule up to $\mathcal{O}(h^2)$ is denoted by “Euler-MacLaurin₂” in table 4. Keeping correction terms up to $\mathcal{O}(h^4)$ (“Euler-MacLaurin₄”) requires the second derivative of $\phi(z = kh)$ which we simply approximate by

$$\phi_k'' = \frac{1}{h^2} [\phi_{k-1} - 2\phi_k + \phi_{k+1}] + \mathcal{O}(h^2). \quad (\text{D.10})$$

Table 4 shows that this gives vastly improved numerical results for the test functions: two or three orders of magnitude more accurate than the simple trapezoidal rule. If there is another point at $z' = 0$ (as in the Green function of the “ray” representation or in the integrand of $I_2(z)$) we simply add the corresponding correction for that point. For the variational calculation we used the “Euler-MacLaurin₂” integration rule with $N = 60$ –120 integration points.

Appendix D.3. Variational equations

We have solved the variational equations by iteration starting with the free solution. Updating during iteration is performed by the simple “linear mixing scheme”

$$y_{\text{in}}^{(n+1)} = \lambda_{\text{mix}} y_{\text{out}}^{(n)} + (1 - \lambda_{\text{mix}}) y_{\text{in}}^{(n)} \quad (\text{D.11})$$

although more elaborate schemes are available (see *e.g.* ref. [44] and references therein). Simply taking $\lambda_{\text{mix}} = 1$ works quite well for high-energy, forward scattering since the potential contribution is suppressed by appropriate powers of $K = k \cos \Theta/2$ in the “aikonal” representation, or k in the “ray” representation. In the former case convergence obviously deteriorates at backward angles and one needs more and more iterations to fulfill the requirement that

$$\left| (X_0 + X_1)^{(n+1)} - (X_0 + X_1)^{(n)} \right| < \epsilon \quad (\text{D.12})$$

which is imposed at fixed impact parameter \mathbf{b} before the iteration is allowed to stop. Typically, we take $\epsilon = 10^{-5}$ or $\epsilon = 10^{-6}$ which results in something like a dozen iterations for small b whereas only one iteration is needed for large (peripheral) values of the impact parameter because the potential for those trajectories is already very feeble. The criterion (D.12) makes sense because the integrand is proportional to $\exp(i(X_0 + X_1 + \dots)) - 1$ so that considerable computing time is saved for trajectories which barely feel the influence of the potential.

Appendix D.4. Gaussian integrals and transforms

Although in all textbooks the Gaussian integral in n dimensions is given as

$$\begin{aligned} I_n(y) &= \int d^n x \exp[-x^T C x + i y^T x] \\ &= \frac{\pi^{n/2}}{\sqrt{\det_n C}} \exp\left[-\frac{1}{4} y^T C^{-1} y\right], \end{aligned} \quad (\text{D.13})$$

this strictly holds only if the matrix C is real symmetric (or Hermitean) positive definite. Recall that this property implies positive eigenvalues λ_j so that the determinant expressed as the product of the eigenvalues

$$\det_n C = \prod_{j=1}^n \lambda_j > 0 \quad (\text{D.14})$$

is positive and eq. (D.13) is unambiguous. However, in our case

$$C = A + iB \quad (\text{D.15})$$

is only *complex symmetric* (the quadratic form $x^T C x$ projects out the symmetric part) and for convergence of the multidimensional Gaussian integral the real part A has to be positive (semi-)definite, *i.e.* $x^T A x \geq 0$ for all x . Under these conditions eq. (D.13) still holds provided the correct sign of the complex square root is chosen. This

is a subtle but important point about which we have not found very much in the literature —except vague remarks that “the sign of the square root is fixed by... analytic continuation” (ref. [45], p. 421). A possible sign change is equivalent to an additional phase π in the exponent of eq. (D.13) and thus very similar to the Maslov phase correction (multiples of $\pi/2$) for a semi-classical propagator when the trajectory of the particle goes through a focal point [46].

In the following we outline how a proper treatment of these “branch corrections” may be obtained. First, we specify which complex square root (which has branchpoints at 0 and ∞) we will use in the following: we choose the cut between these branchpoints along the negative real axis and define the principal square root of a complex number z as the one with a positive real part, *i.e.*

$$\sqrt{z} := \sqrt{|z|} \exp\left(\frac{1}{2} i \arg z\right), \quad |\arg z| < \pi. \quad (\text{D.16})$$

This is also the value returned by the subroutine for the complex square root in the numerical implementation. Then we assume that the complex symmetric matrix C may be diagonalized by a complex orthonormal transformation

$$C = O D O^T \quad \text{with } O^T O = O O^T = 1 \quad (\text{D.17a})$$

and

$$D = \text{diag}(\lambda_1, \lambda_2 \dots \lambda_n) \quad (\text{D.17b})$$

so that

$$\begin{aligned} I_n(y) &= \int d^n x' \exp\left[-\sum_{j=1}^n \lambda_j x_j'^2 + i \sum_{j=1}^n (y^T O)_j x_j'\right] \\ &= \prod_{j=1}^n \left(\int dx_j'' \exp\left[-\lambda_j x_j''^2 - \frac{(y^T O)_j^2}{4\lambda_j}\right] \right) \end{aligned} \quad (\text{D.18})$$

because the Jacobian of an orthonormal transformation is unity¹⁰. Due to a theorem by Bendixson (see eq. (6.9.15) in ref. [47]) the real parts of the complex eigenvalues

$$\text{Re } \lambda_j \geq 0 \quad (\text{D.19})$$

remain nonnegative when the eigenvalues of the real part of C are assumed to be (semi-)positive definite. In other words: we can write

$$\lambda_j = r_j e^{i\phi_j}, \quad \text{with } |\phi_j| < \frac{\pi}{2}. \quad (\text{D.20})$$

¹⁰ Lacking an explicit proof we here assume —as done tacitly in all textbooks— that the complex orthonormal transformation of the original co-ordinates x_i and the linear shift leads to integration paths for the transformed co-ordinates x_j'' in the complex plane which can be safely rotated back to the real axis. Analytic continuation of the real result faces a similar difficulty as one can only perform it from a *region* in the complex plane and not from the real axis.

Thus, each integral in the product of eq. (D.18) is convergent and we obtain

$$\begin{aligned} I_n(y) &= \left(\prod_{j=1}^n \sqrt[4]{\frac{\pi}{\lambda_j}} \right) \exp \left[-\frac{1}{4\lambda_j} (y^T O)_j^2 \right] \\ &= \pi^{n/2} \left(\prod_{j=1}^n \frac{1}{\sqrt[4]{\lambda_j}} \right) \exp \left[-\frac{1}{4} \sum_{j=1}^n y_j (O D^{-1} O^T)_j y_j \right] \\ &= \pi^{n/2} \left(\prod_{j=1}^n \frac{1}{\sqrt[4]{\lambda_j}} \right) \exp \left(-\frac{1}{4} y^T C^{-1} y \right) \end{aligned} \quad (\text{D.21})$$

as expected. However, it is important to note that the prefactor is not given by the inverse square root of the determinant of C but by the product of the inverse square roots of the complex eigenvalues (D.20). This may be different¹¹ depending on the value of

$$\Phi^{(n)} = \sum_{j=1}^n \phi_j, \quad |\Phi^{(n)}| < n \frac{\pi}{2}. \quad (\text{D.22})$$

Then,

$$\begin{aligned} \prod_{j=1}^n \frac{1}{\sqrt[4]{\lambda_j}} &= \frac{1}{\sqrt[4]{\det_n C}} \exp(-i n_{\text{br}}(C) \pi) = \\ &= \frac{1}{\sqrt[4]{|\det_n C|}} \exp \left(-\frac{i}{2} \arg \det_n C - i n_{\text{br}}(C) \pi \right), \end{aligned} \quad (\text{D.23})$$

where the “branch number” is given by

$$n_{\text{br}}(C) = \left[\frac{|\Phi^{(n)}| + \pi}{2\pi} \right] \quad (\text{D.24})$$

and $[x]$ is the maximum integer not greater than x . $n_{\text{br}} = 0, 2, \dots$ denotes the principal branch of the square root and $n_{\text{br}} = 1, 3, \dots$ the other, negative branch. From eq. (D.22) we have the following bound for a $(n \times n)$ complex symmetric matrix C with nonnegative real part

$$n_{\text{br}}(C) < \left\lceil \frac{n+2}{4} \right\rceil. \quad (\text{D.25})$$

Note that in contrast to the Maslov correction this additional phase is not discontinuous but rather corrects the phase jump when crossing the (arbitrary) branch cut of the complex square root. In this way the analytic continuation of the result (D.13) is achieved. As an example take $\Phi = \pi + \epsilon$ to obtain $-\frac{1}{2} \arg \det C - n_{\text{br}} \pi = -\pi/2 + |\epsilon|/2$ for $\epsilon < 0$ ($n_{\text{br}} = 0$, above the cut) and $\pi/2 - \epsilon/2 - \pi = -\pi/2 - \epsilon/2$ for $\epsilon > 0$ ($n_{\text{br}} = 1$, below the cut).

After these preliminaries we can now calculate the general Gaussian transform required in our variational approach. This is particularly straightforward and simple for

¹¹ Take the simple example: $n = 3$, $\lambda_j \equiv \lambda = i + 0^+$. Then $\det_3 = -i - 0^+$, $\sqrt[4]{\det_3} = (1-i)/\sqrt{2}$ but $(\sqrt[4]{\lambda})^3 = -(1-i)/\sqrt{2}$.

a Gaussian potential: from

$$\begin{aligned} \tilde{V}_\sigma(\mathbf{p}) &= \tilde{V}(\mathbf{p}) \cdot \exp \left(-\frac{1}{2} p_i \sigma_{ij} p_j \right) = \\ &= V_0 (\pi R^2)^{3/2} \exp \left[-\frac{R^2}{4} p_i (\delta_{ij} + 2\sigma_{ij}/R^2) p_j \right] \end{aligned} \quad (\text{D.26})$$

it follows by inverse Fourier transformation:

$$\begin{aligned} V_\sigma(\mathbf{x}) &= V_0 \pi^{3/2} R^3 \int \frac{d^3 p}{(2\pi)^3} \exp \left[-\frac{R^2}{4} p_i C_{ij} p_j - i p_i x_i \right] \\ &= \frac{V_0}{\sqrt[4]{\det_3 C}} \exp[-\alpha x_i C_{ij}^{-1} x_j - i n_{\text{br}}(C) \pi], \end{aligned} \quad (\text{D.27})$$

where

$$C_{ij} = \delta_{ij} + 2\alpha \sigma_{ij}, \quad \alpha = \frac{1}{R^2}. \quad (\text{D.28})$$

is a complex symmetric (3×3) -matrix whose real part should be positive (semi-)definite. Unfortunately we were unable to verify this property analytically for our variational solutions but did not encounter any numerical instabilities (which would be caused by a blow-up of V_σ) during the iterative solution of the variational equations if z_{max} was not too large. Determinant and inverse of the (3×3) -matrix C are known from elementary calculus but we have not found a simple but reliable method to determine the “branch number” n_{br} which in principle — according to eq. (D.25) — could be nonzero even in this case. A method of “branch tracking” has been described in ref. [48] but we used a less elegant, brute-force approach in which the complex eigenvalues were determined numerically with the NAG routine F02GBF and the prefactor was calculated as a product of the square roots of these. As a by-product it was confirmed that the real parts of the eigenvalues were always positive. After evaluation of the Gaussian transform of the potential the Jacobian and the Hessian then simply follow by differentiation:

$$(J_\sigma)_i \equiv \partial_i V_\sigma(\mathbf{x}) = -2\alpha (C^{-1})_{ik} x_k V_\sigma(\mathbf{x}), \quad (\text{D.29})$$

$$(H_\sigma)_{ij} \equiv \partial_i \partial_j V_\sigma(\mathbf{x}) = -2\alpha \left[(C^{-1})_{ij} \right. \quad (\text{D.30})$$

$$\left. -2\alpha (C^{-1})_{ik} x_k (C^{-1})_{jl} x_l \right] V_\sigma(\mathbf{x}). \quad (\text{D.31})$$

For the calculation of the second cumulant we also need the *double* Gaussian transform

$$I_6 := \int d^3 p_1 d^3 p_2 \exp[-\mathbf{p}^T C \mathbf{p} + i \mathbf{x} \cdot \mathbf{p}], \quad (\text{D.32})$$

where

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{pmatrix} \quad (\text{D.33})$$

is a complex symmetric (6×6) -matrix (see eq. (3.27)) and

$$\mathbf{p} = \begin{pmatrix} \mathbf{p}_1 \\ \mathbf{p}_2 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} \quad (\text{D.34})$$

are 6-dimensional (column) vectors. Determinant, inverse and branching number have been evaluated as in the

3-dimensional case by calculating the complex eigenvalues — a procedure which increased the execution time of the program considerably. We found that (under our kinematical conditions) no branch crossing occurred in the 3-dimensional calculation of the Gaussian transform of the potential but the sign change of the complex square root was essential to obtain the correct results in the 6-dimensional case (calculation of the second cumulant).

Appendix D.5. Calculation of Ω

Arising from a functional determinant the quantity Ω poses a particular problem for numerical evaluation. Several approaches are possible.

First, one may employ the classic method of Gel'fand and Yaglom [49] (already contained in textbooks, *e.g.* in ref. [33], Chapt. 6) to calculate a functional determinant as solution of an initial value differential equation. Indeed, defining

$$\Omega_0 := \frac{1}{2} \text{Tr} \ln (1 - \Sigma_0 H_\sigma) \quad (\text{D.35})$$

(so that $\Omega = \Omega_0 + \text{Tr}(\Sigma H_\sigma)/2$) its exponential is given as ratio of two functional determinants

$$\exp(2\Omega_0) = \frac{\text{Det}(-\partial_t^2 - H_\sigma/m)}{\text{Det}(-\partial_t^2)} \quad (\text{D.36})$$

and one may apply the Gel'fand-Yaglom procedure to evaluate it. However, the boundary conditions for the eigenfunctions $f(t)$ of the differential operators in eq. (D.36) are not of Dirichlet type as in the standard method but (in the “aikonal” case, cf. eqs. (3.32a) and (3.32b)) of the form

$$\begin{aligned} \lim_{T \rightarrow \infty} \left\{ f(T) + f(-T) - T \left(\dot{f}(t) - \dot{f}(-T) \right) \right\} &= 0, \\ \lim_{T \rightarrow \infty} \left\{ \dot{f}(t) + \dot{f}(-T) \right\} &= 0. \end{aligned} \quad (\text{D.37})$$

Although Kirsten and McKane [50] recently have generalized the classic procedure to more general boundary conditions like (D.37) we do not follow this approach since simpler alternatives are available.

These include, second, the calculation of Ω as power series in either ΣH_σ or $\Sigma_0 H_\sigma$:

$$\Omega = \frac{1}{2} \text{Tr} [-\ln(1 + \Sigma H_\sigma) + \Sigma H_\sigma] \quad (\text{D.38})$$

$$= \frac{1}{2} \text{Tr} \sum_{n=2}^{\infty} \frac{(-)^n}{n} \text{Tr} (\Sigma H_\sigma)^n, \quad (\text{D.39})$$

$$\Omega = \frac{1}{2} \text{Tr} \left[\ln(1 - \Sigma_0 H_\sigma) + \frac{1}{1 - \Sigma^{(0)} H_\sigma} - 1 \right] \quad (\text{D.40})$$

$$= \frac{1}{2} \text{Tr} \sum_{n=2}^{\infty} \left(1 - \frac{1}{n} \right) \text{Tr} (\Sigma_0 H_\sigma)^n. \quad (\text{D.41})$$

If the variational equations are fulfilled this should give identical results as should the “mixed” form

$$\Omega = \frac{1}{2} \text{Tr} [\ln(1 - \Sigma_0 H_\sigma) + \Sigma H_\sigma] \quad (\text{D.42})$$

$$= \frac{1}{2} \left[- \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr} (\Sigma_0 H_\sigma)^n + \text{Tr} (\Sigma H_\sigma) \right] \quad (\text{D.43})$$

in which $1/(1 - \Sigma_0 H_\sigma) - 1 = \Sigma H_\sigma$ has been used. Note that in the “aikonal” case the sum also begins at $n = 2$ since $\Sigma_0(t, t) = 0$. If the variational equations are solved by iteration it is consistent to evaluate the various sums in eqs. (D.39), (D.41) and (D.43) up to $n = \#$ of iterations since each term is suppressed by an additional power of K or k — if the iteration converges so will the power series expansion for Ω . One should keep in mind that this procedure only works as long as $KR \gg 1$ or $kR \gg 1$, *i.e.* at high energies and not too large scattering angles.

Third, one may evaluate the functional determinant as a $(3 \times n_g \times n_e)$ -dimensional ordinary determinant on the grid as one has discretized the time (or z -co-ordinate) for the solution of the variational equations and the various integrals anyway. The NAG program F03ADF was used for this purpose.

Finally, the complex eigenvalues λ_j of the matrix $1 + \Sigma H_\sigma$ may be calculated (with the help of the NAG routine F02GBF) so that from eq. (D.38)

$$\Omega = \frac{1}{2} \sum_j [\lambda_j - 1 - \ln \lambda_j]. \quad (\text{D.44})$$

This also checks whether a “branch crossing” may have occurred which is unlikely under these kinematic conditions as ΣH_σ remains “small” and the power series of the logarithm is well converging. Indeed, we found no case where the square root of the determinant was different from the product of the square roots of the eigenvalues.

Table 5 compares the results of the different methods in the “aikonal” representation at a fixed value of the impact parameter. One observes excellent agreement between the different methods.

Also included is a test at high energies where according to eqs. (3.46) and (3.44) the phases and the fluctuation term can be described by the (much simpler) “aikonal” phases. These have been worked out in ref. [22] for spherically symmetric potentials (see eqs. (4.98), (4.99), (4.104) and (4.111) therein) so that the corresponding expressions for a Gaussian potential read

$$\chi_{\text{AI}}^{(0)} = -C \frac{\sqrt{\pi}}{2} e^{-y}, \quad (\text{D.45})$$

$$\chi_{\text{AI}}^{(1)} = -\frac{C^2}{KR} \frac{1}{8} \sqrt{\frac{\pi}{2}} (1 - 4y) e^{-2y}, \quad (\text{D.46})$$

$$\begin{aligned} \chi_{\text{AI}}^{(2)} = -\frac{C^3}{(KR)^2} \frac{1}{16} \sqrt{\frac{\pi}{3}} \left[1 - (12 + \sqrt{3}\pi) y \right. \\ \left. + (12 + 2\pi/\sqrt{3}) y^2 \right] e^{-3y}, \end{aligned} \quad (\text{D.47})$$

Table 5. Comparison of values for the fluctuation term (functional determinant) Ω calculated in different ways (see text) at $b/R = 1$ for the Gaussian potential (4.1). Parameters of the calculation: $z_{\max}/R = 5$, $(n_g, n_e) = (32, 2)$, $\epsilon = 10^{-5}$, $\lambda_{\text{mix}} = 1$. Results for two values of the energy and the potential strength are displayed to allow comparison with the “aikonal” phases to which the total sum $X_0 + X_1 + i\Omega$ should tend in the high-energy limit.

	$KR = 4, 2mV_0R^2 = -4$		$KR = 8, 2mV_0R^2 = -8$	
	(# of iterations = 5)		(# of iterations = 4)	
	Re	Im	Re	Im
Ω , eq. (D.39)	-4.1931 (-3)	-6.2753 (-4)	-9.6244 (-4)	-4.3797 (-5)
Ω , eq. (D.41)	-4.1930 (-3)	-6.2751 (-4)	-9.6258 (-4)	-4.3810 (-5)
Ω , eq. (D.43)	-4.1935 (-3)	-6.2748 (-4)	-9.6243 (-4)	-4.3812 (-5)
Ω , eq. (D.38)	-4.1934 (-3)	-6.2747 (-4)	-9.6246 (-4)	-4.3814 (-5)
Ω , eq. (D.42)	-4.1932 (-3)	-6.2756 (-4)	-9.6247 (-4)	-4.3799 (-5)
Ω , eq. (D.44)	-4.1932 (-3)	-6.2756 (-4)	-9.6247 (-4)	-4.3799 (-5)
$X_0 + X_1$	3.4056 (-1)	8.1621 (-3)	3.3382 (-1)	1.8965 (-3)
$X_0 + X_1 + i\Omega$	3.4118 (-1)	3.9688 (-3)	3.3386 (-1)	9.3403 (-4)
$\chi_{\text{AI}}^{(0)} + \chi_{\text{AI}}^{(1)} + \chi_{\text{AI}}^{(2)}$	3.4176 (-1)	0.	3.3394 (-1)	0.
$i\omega_{\text{AI}}^{(2)}$	0.	3.3216 (-3)	0.	8.3041 (-4)

Table 6. Test of the Feynman-Hellmann relation (D.49) for fixed $b/R = 1$ in the “aikonal” representation and fixed $b_x/R = 0.6$, $b_y/R = 0.8$ in the “ray” representation. In the latter case the scattering angle has been fixed at $\theta = 60^\circ$ with the momentum transfer along the x -axis. Accuracy parameters for the numerical solution of the variational equations are as in table 5 and the integration over the potential strength was performed by Gauss-Legendre integration with n_{FH} points.

		“aikonal”		“ray”	
		Re	Im	Re	Im
r.h.s. of eq. (D.49)	$n_{\text{FH}} = 8$	3.41182 (-1)	3.96843 (-3)	2.50889 (-1)	3.38986 (-2)
r.h.s. of eq. (D.49)	$n_{\text{FH}} = 12$	3.41182 (-1)	3.96839 (-3)	2.50889 (-1)	3.38987 (-2)
$X_0 + X_1 + i\Omega$		3.41183 (-1)	3.96882 (-3)	2.50889 (-1)	3.38993 (-2)

$$\omega_{\text{AI}}^{(2)} = -\frac{C^2}{(KR)^2} \frac{\pi}{8} (1 - 4y + 2y^2) e^{-2y}, \quad (\text{D.48})$$

with $C = 2mV_0R^2/(KR)$ and $y = b^2/R^2$.

Good quantitative agreement is observed which becomes better at higher energies as expected. Note that at $KR = 8$ the strength has also been changed to keep $mV_0/K = \text{constant}$. According to eqs. (3.46), (3.49) the difference between $X_0 + X_1 + i\Omega$ and $\sum_{k=0}^2 \chi_{\text{AI}}^{(k)} + i\omega_{\text{AI}}^{(2)}$ then should decrease as $1/K^3$. Indeed, a closer look at the numerical values in table 5 shows that this difference decreases by a factor 7.9 in the real part and a factor 6.3 in the imaginary part when doubling the energy which is in reasonable agreement with the expected factor $(8/4)^3 = 8$.

Appendix D.6. Test of the Feynman-Hellmann theorem

As explained in sect. 3.6 the variational impact-parameter S -matrix should fulfill additional relations since its ingre-

dients are solutions of the variational equations. Here we will use the dependence (3.55) on the coupling strength V_0 to test our numerical solutions. Upon integrating we should have

$$X_0 + X_1 + i\Omega \Big|_V = \int_0^1 d\lambda \frac{1}{\lambda} X_0 \Big|_{V \rightarrow \lambda V} \quad (\text{D.49})$$

for fixed \mathbf{b} (and scattering angle).

The r.h.s. of this relation may be evaluated by simple Gauss-Legendre integration (which has the advantage of avoiding the point $\lambda = 0$) over the “phase” X_0 at different strength of the potential. As the integrand is a smooth function of the potential strength very few Gaussian points are necessary to achieve a stable result which is in excellent agreement with the l.h.s. of eq. (D.49). This is displayed in table 6, both for the “aikonal” and the “ray” representation and constitutes a rather stringent test that our numerical scheme for solving the variational equations and for calculating the stationary values is correct.

Note added in proofs. The correct mathematical framework to derive the Gaussian integral with complex symmetric matrices is the theory of “pencils” [51] (called “Büschel” in the German nomenclature [52]) of quadratic forms which avoids the problems indicated in footnote¹⁰. Fortunately, this approach leads to the same result and procedures as used in appendix D.4.

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