Gaussian-Wave-Packet Dynamics in Uniform Magnetic and Quadratic Potential Fields*

H. Y. Kim† and J. H. Weiner
Brown University, Providence, Rhode Island 02912
(Received 24 July 1972)

For the case of uniform magnetic field and a potential quadratic in its coordinates an electron state originally represented by a Gaussian wave packet remains Gaussian in its subsequent evolution. Under these conditions the state is completely characterized by the first- and second-order quantum means, that is, quantities such as $\langle q_i \rangle$, $\langle p_i \rangle$ and $\langle q_i p_j \rangle$, $\langle p_i p_j \rangle$, respectively. A tensor-product relationship is shown to exist between the problem of the determination of the second- and first-order means which facilitates the solution. Two problems are treated in detail: (i) an isotropic wave packet in an isotropic potential well and (ii) the dynamics of a wave packet on a quadratic saddle point. In the former case, the wave packet "spins" and its radius pulsates as its mean follows the classical trajectory. In the second the magnetic field effect on tunneling through such barriers is studied and found to be small at attainable field strengths unless the effective electronic mass is very small. A method for the numerical solution for the time-dependent Schrödinger equation, termed the particle method and based on the hydrodynamic analogy to that equation, is here extended to include magnetic fields. It is applied to the two problems just described and found to agree well with the analytical solutions.

I. INTRODUCTION

We are concerned in this paper with time-dependent solutions for wave-packet states of an electron in a constant uniform magnetic field and subject as well to a potential which is quadratic in the coordinates.

This problem was suggested by a theory of quantum-rate processes in solids[1-3] in which a small component (e.g., an impurity atom) that is in a trapped localized state and in thermal equilibrium with the rest of the solid is represented by an appropriate ensemble of Gaussian wave packets. The rate with which such components leave this localized state by either passing over a potential barrier or by tunneling is determined in this theory by computing the dynamical behavior of such wave packets according to the time-dependent Schrödinger equation. In this way, thermal activation and tunneling are both treated in a unified way. Although the theory was originally developed to describe light-atom diffusion processes, it appears that a similar viewpoint may be useful in the study of electron-hopping conduction[4] in amorphous solids. The present work is then a step towards the incorporation of magnetic field effects in such a study.

In this paper, however, we do not pursue the rate-theory aspects of the process but focus on the mathematical problem of the wave-packet dynamics under the stated conditions. By considering a potential quadratic in the coordinates we are able to treat the wave-packet dynamics both when it is trapped in a potential well and when it is moving on a saddle point representing the barrier separating two wells.

This class of problem has a long history with the earliest treatment apparently that of Darwin[5] in his analysis of Landau diamagnetism. The quadratic potential, taken as isotropic, was used by him as a device to localize the electron, and ultimately in the analysis the potential strength was allowed to vanish. The work of Husimi[6] similarly employed an (vanishing) isotropic potential well.

This class of problems has been reexamined recently by a number of authors using, in general, quantum-mechanical techniques and concepts of current interest. For example, the coherent-state formalism has been utilized by Malkin and Man'ko,[7] Feldman and Kahn,[8] and Tam.[9] Papadopoulos[10] obtains the propagator of the Schrödinger equation for a harmonically bound particle in a magnetic field by path-integral methods. The work of Langebein,[11] who treats the case of electron-wave-packet dynamics when subject to a lattice potential should also be noted.

In this paper we present still another approach to the problem, one which represents an extension to include magnetic field effects of a method previously presented[3] for the case with magnetic field absent. We confine attention to wave packets which are initially Gaussian and remain so under the stated conditions (uniform magnetic field and quadratic potential). These are more general than coherent-state wave packets since their shape need not be time independent, and they include the latter as a special case. These Gaussian states [defined in Eqs. (2.3) and (2.4)] are, except for a phase factor, completely characterized at any instant of time by their associated first- and second-order quantum means and therefore the solution of the time-dependent Schrödinger equation may be re-

placed by the solution of the system of ordinary differential equations (derived in Sec. II) which these means satisfy.[3] In Sec. III a tensor-product relationship is shown to exist between the eigenvalue problem for the second-order means and that for the first-order means, a relationship which simplifies the solution of the former problem.

While the discussion until this point is valid for the three-dimensional case, it is specialized in Sec. IV to treat only the wave-packet motion in the plane perpendicular to the magnetic field $\vec{B}$ with $\vec{B}$ in one of the principal directions of the quadratic potential $V(\vec{q})$. For the case in which $V(\vec{q})$ represents an isotropic potential well and for an isotropic Gaussian wave packet, the solution is obtained in explicit form for arbitrary field strength B. The wave-packet mean follows the classical motion while the wave-packet "radius" pulsates; for suitable initial conditions the "radius" remains constant and the solution reduces to the coherent-state case treated by Feldman and Kahn.[8] For the general case with anisotropic quadratic potential $V(\vec{q})$ and anisotropic wave packet, the explicit form of the solution becomes very cumbersome, and we give here only the approximate form it assumes, valid to first order in B.

In Sec. V we turn to the question of the numerical solution of problems of this type using an approach, termed the particle method,[2,12] which is based on the hydrodynamic analogy to the time-dependent Schrödinger equation. This method is readily extended to include magnetic field effects and is applied in this section to the case of the isotropic potential well and to the problem of a wave packet moving on a quadratic saddle point; the numerical results agree well with the analytical solution of Sec. IV, and for the saddle point show the nature of the magnetic field effect upon tunneling through such a barrier. Some concluding remarks are presented in Sec. VI.

II. PROBLEM FORMULATION

The problem we are concerned with is the dynamics of a Gaussian wave packet representing an electron subject to a potential $V(\vec{q})$ (not necessarily solely electromagnetic in origin) which is quadratic in the coordinates $\vec{q}$, and to a constant uniform magnetic field $\vec{B}$. The treatment is nonrelativistic with spin neglected so that the time-dependent Schrödinger equation for the wave function $\psi(\vec{q},t)$ takes the form

$$\{\tfrac{1}{2}[-i\nabla-\vec{A}(\vec{q})]^2+V(\vec{q})\}\psi(\vec{q},t)=i\frac{\partial\psi(\vec{q},t)}{\partial t}. \quad (2.1)$$

Here, and throughout the paper, atomic units, $\hbar=e=m=1$, are employed. $\vec{A}(\vec{q})$ is the magnetic vector potential for which we use the symmetric gauge:

$$\vec{A}(\vec{q})=\tfrac{1}{2}(\vec{B}\times\vec{q}). \quad (2.2)$$

The magnetic field is defined relative to the speed of light c so that the cyclotron frequency is equal to B.

Under the stated conditions it may be verified by direct substitution into Eq. (2.1) that an initially Gaussian wave packet remains Gaussian[13] for all subsequent time. That is, the wave function $\psi(\vec{q},t)$ may be written in the form

$$\psi(\vec{q},t)=R(\vec{q},t)\,e^{iS(\vec{q},t)}, \quad (2.3)$$

where

$$R=(2\pi)^{-N/4}|\chi|^{-1/4}e^{-(\chi^{-1}_{ij}\hat{q}_i\hat{q}_j)/4},$$

$$S=\tfrac{1}{2}a_{ij}\hat{q}_i\hat{q}_j+b_i\hat{q}_i+c. \quad (2.4)$$

The notation introduced in Eq. (2.4) is as follows: q_i is the ith component of $\vec{q}$ with respect to a rectangular Cartesian coordinate system; $\langle q_i\rangle(t)$ is its quantum mean; $\hat{q}_i=q_i-\langle q_i\rangle$, $|\chi|$ is the determinant of the matrix $\underline{\chi}$ [the covariance matrix of the Gaussian distribution—see the first line of Eq. (2.5)] with components $\chi_{ij}(t)$; χ^{-1}_{ij} are the components of $\underline{\chi}^{-1}$, and a_{ij}, b_i, and c are functions of time. The summation convention $i=1,\ldots,N$ is employed; the general discussion of Secs. II and III are applicable for $N=3$, while in the subsequent particular calculations $\vec{B}$ is taken to lie in the q_3 direction and attention is confined to the wave-packet motion in the q_1, q_2 plane. In the latter case, $N=2$. A straightforward but tedious method of finding the ordinary differential equations that χ_{ij}, a_{ij}, and b_i must satisfy is substitution of ψ as defined in Eq. (2.3) into the time-dependent Schrödinger equation, Eq. (2.1), and equating to zero the coefficients of the different powers of q_i (0, 1, and 2) which appear. [It is readily verified that only these powers appear since $V(\vec{q})$ is quadratic and $\vec{B}$ is uniform.] An alternate approach which reveals the structure of the problem more clearly is to note first (as may be verified by direct computation) that the quantities χ_{ij}, a_{ij}, and b_i are related to quantum means associated with ψ as follows:

$$\chi_{ij}=\langle\hat{q}_i\hat{q}_j\rangle=\langle q_iq_j\rangle-\langle q_i\rangle\langle q_j\rangle,$$

$$2a_{ij}\chi_{ik}=\langle\hat{q}_k\hat{p}_j+\hat{p}_j\hat{q}_k\rangle, \quad (2.5)$$

$$b_i=\langle p_i\rangle,$$

where p_i are the momenta and $\hat{p}_i=p_i-\langle p_i\rangle$. The determination of these quantum means [or others, Eqs. (2.14) and (2.15), which may be used to define them] is therefore sufficient to determine ψ to within an arbitrary phase factor and this is the approach which we adopt here.

The determination of the ordinary differential equations which the quantum means satisfy rests on the basic equation for an arbitrary operator A,

$$\frac{d\langle A\rangle}{dt}=\frac{1}{i}\langle[A,H]\rangle+\left\langle\frac{\partial A}{\partial t}\right\rangle\ , \tag{2.6}$$

where

$$H=\tfrac{1}{2}(p_i-A_i)(p_i-A_i)+\tfrac{1}{2}V_{ij}q_iq_j$$

$$=\tfrac{1}{2}\pi_i\pi_i+\tfrac{1}{2}V_{ij}q_iq_j \tag{2.7}$$

is the Hamiltonian of the system. In the latter form of the Hamiltonian we have introduced the kinetic momentum $\vec{\pi}$ with components

$$\pi_i=p_i-A_i\ , \tag{2.8}$$

where A_i are the components of the vector potential $\vec{A}$. For the uniform magnetic field considered here we note from Eq. (2.2) that $\vec{A}$ is linear in $\vec{q}$, that is,

$$A_i=\tfrac{1}{2}\epsilon_{ijk}B_jq_k=A_{ik}q_k \tag{2.9}$$

with $A_{ik}=-A_{ki}$.

The equations governing $\langle q_i\rangle$ and $\langle\pi_i\rangle$ (Ehrenfest's theorem) are readily derived from Eq. (2.6) as

$$\frac{d\langle q_i\rangle}{dt}=\langle\pi_i\rangle\ ,$$
$$\frac{d\langle\pi_i\rangle}{dt}=-(V_{ik}\langle q_k\rangle+2A_{ik}\langle\pi_k\rangle)\ . \tag{2.10}$$

It follows from Eqs. (2.10) that, under the stated conditions of quadratic potential V and uniform magnetic field, the quantum means follow the classical motion. We next consider two operators A and B which do not depend explicitly on time and define their deviators $\hat{A}$, $\hat{B}$ as

$$\hat{A}=A-\langle A\rangle\ ,\quad \hat{B}=B-\langle B\rangle\ . \tag{2.11}$$

It is then readily verified that

$$\langle\hat{A}\hat{B}\rangle=\langle AB\rangle-\langle A\rangle\langle B\rangle \tag{2.12}$$

and

$$\frac{d\langle\hat{A}\hat{B}\rangle}{dt}=\frac{1}{i}\langle[\hat{A}\hat{B},H]\rangle\ . \tag{2.13}$$

In deriving Eq. (2.13) from Eq. (2.6), use is made of the fact that the time-dependent portions of $\hat{A}$ and $\hat{B}$, namely, $\langle A\rangle$ and $\langle B\rangle$, also satisfy Eq. (2.6). By use of Eq. (2.13) we may then derive the following autonomous set of first-order ordinary differential equations for the quantities $\langle\hat{q}_i\hat{q}_j\rangle$, $\langle\hat{q}_i\hat{\pi}_j\rangle$, $\langle\hat{\pi}_i\hat{q}_j\rangle$, and $\langle\hat{\pi}_i\hat{\pi}_j\rangle$:

$$\frac{d\langle\hat{q}_i\hat{q}_j\rangle}{dt}=\langle\hat{q}_i\hat{\pi}_j\rangle+\langle\hat{\pi}_i\hat{q}_j\rangle\ ,$$

$$\frac{d\langle\hat{q}_i\hat{\pi}_j\rangle}{dt}=\langle\hat{\pi}_i\hat{\pi}_j\rangle-2A_{jk}\langle\hat{q}_i\hat{\pi}_k\rangle-V_{jk}\langle\hat{q}_i\hat{q}_k\rangle\ ,$$

$$\frac{d\langle\hat{\pi}_i\hat{q}_j\rangle}{dt}=\langle\hat{\pi}_i\hat{\pi}_j\rangle-2A_{ik}\langle\hat{\pi}_k\hat{q}_j\rangle-V_{ik}\langle\hat{q}_k\hat{q}_j\rangle\ ,$$

$$\frac{d\langle\hat{\pi}_i\hat{\pi}_j\rangle}{dt}=-2A_{jk}\langle\hat{\pi}_i\hat{\pi}_k\rangle-V_{jk}\langle\hat{\pi}_i\hat{q}_k\rangle$$
$$-2A_{ik}\langle\hat{\pi}_k\hat{\pi}_j\rangle-V_{ik}\langle\hat{q}_k\hat{\pi}_i\rangle\ . \tag{2.14}$$

The operators $\hat{q}_i\hat{\pi}_j$ and $\hat{\pi}_j\hat{q}_i$ appearing in the system of Eqs. (2.14) are not individually Hermitian, and it is only the sum $\langle\hat{q}_i\hat{\pi}_j\rangle+\langle\hat{\pi}_j\hat{q}_i\rangle=\langle\hat{q}_i\hat{\pi}_j+\hat{\pi}_j\hat{q}_i\rangle$ which is real. Similarly, $\hat{\pi}_i\hat{\pi}_j$ is not Hermitian and only $\langle\hat{\pi}_i\hat{\pi}_j+\hat{\pi}_j\hat{\pi}_i\rangle$ is real. Nevertheless, it is convenient for future purposes to write the system in the form shown. We also note that

$$\langle\hat{q}_i\hat{\pi}_j+\hat{\pi}_j\hat{q}_i\rangle=\langle\hat{q}_i\hat{p}_j+\hat{p}_j\hat{q}_i\rangle-2A_{jk}\langle\hat{q}_i\hat{q}_k\rangle\ , \tag{2.15}$$

so that the determination of the means appearing in Eqs. (2.14) supply as well the means needed in Eqs. (2.5).

III. RELATION BETWEEN FIRST- AND SECOND-ORDER MEANS

We will, in the following, refer to quantum means such as $\langle q_i\rangle$ and $\langle\pi_i\rangle$ as first order and to means such as $\langle\hat{q}_i\hat{q}_j\rangle$, $\langle\hat{q}_i\hat{\pi}_j\rangle$, etc. as second order. We next derive a relation between the systems of equations for the second-order means [Eqs. (2.14)] and the system for the first-order means [Eqs. (2.10)]; this relation facilitates the determination of the second-order means.

In order to make the derivation more compact, we introduce the notation $\vec{X}$ for the six-dimensional vector whose components X_k, $k=1,\ldots,6$ are the operators q_1, q_2, q_3, π_1, π_2, π_3. Then, since H is quadratic in these quantities,

$$(1/i)[X_k,H]=C_{kl}X_l\ , \tag{3.1}$$

where the constants C_{kl} are the elements of the 6×6 matrix $\underline{C}$,

$$\underline{C}=\begin{pmatrix}0 & \underline{I}_3\\ -\underline{V} & -2\underline{A}\end{pmatrix}\ . \tag{3.2}$$

Here, $\underline{V}$ and $\underline{A}$ are the 3×3 matrices with elements V_{ij}, A_{ij} and $\underline{I}_3$ is the 3×3 identity matrix. In this notation Eqs. (2.10) for the first-order means may be rewritten

$$\frac{d\langle X_k\rangle}{dt}=C_{kl}\langle X_l\rangle\ . \tag{3.3}$$

We next turn to the second-order means. From Eq. (2.13), we find

$$\frac{d\langle\hat{X}_k\hat{X}_l\rangle}{dt}=\frac{1}{i}\langle[\hat{X}_k\hat{X}_l,H]\rangle$$
$$=\frac{1}{i}\langle\hat{X}_k[\hat{X}_l,H]+[\hat{X}_k,H]\hat{X}_l\rangle\ ,$$

or, from Eq. (3.1),

$$\frac{d\langle\hat{X}_k\hat{X}_l\rangle}{dt}=C_{lm}\langle\hat{X}_k\hat{X}_m\rangle+C_{km}\langle\hat{X}_m\hat{X}_l\rangle\ . \tag{3.4}$$

In the usual manner, we seek solutions to Eqs.

(3.3) and (3.4) in the form

$$\langle X_k\rangle(t)=F_k^{(1)}e^{\lambda^{(1)}t}\,,\quad \langle \hat{X}_k\hat{X}_l\rangle(t)=F_{kl}^{(2)}e^{\lambda^{(2)}t}\,, \tag{3.5}$$

where the superscripts (1) and (2) emphasize that the quantities refer to first- and second-order means, respectively. Substitution of Eqs. (3.5) into (3.3) and (3.4) leads to the algebraic equations

$$C_{kl}F_l^{(1)}=\lambda^{(1)}F_k^{(1)}\,, \tag{3.6}$$

$$C_{km}F_{ml}^{(2)}+C_{lm}F_{km}^{(2)}=\lambda^{(2)}F_{kl}^{(2)}\,. \tag{3.7}$$

The vectors $\vec{F}^{(1)}$ are elements of the six-dimensional vector space R^6. The vectors $\vec{F}^{(2)}$ are components of a 36-dimensional vector space that is convenient to regard here as the tensor product[14] $R^6\otimes R^6$. The 6×6 matrix $\underline{C}$ can then be extended to act on $R^6\otimes R^6$ as either $\underline{C}\otimes\underline{I}_6$ or $\underline{I}_6\otimes\underline{C}$ (with $\underline{I}_6$ the 6×6 identity matrix), and Eq. (3.7) can be rewritten in the form

$$[(\underline{C}\otimes\underline{I}_6)+(\underline{I}_6\otimes\underline{C})]\,\vec{F}^{(2)}=\lambda^{(2)}\vec{F}^{(2)}\,. \tag{3.8}$$

Let $\lambda_\alpha^{(1)}$, $\alpha=1,\ldots,6$ be the eigenvalues of $\underline{C}$ with $\vec{F}_\alpha^{(1)}$ the corresponding (linearly independent) eigenvectors. Then, it can be verified by direct substitution that 36 linearly independent solutions of Eq. (3.8) are

$$\vec{F}_{\alpha\beta}^{(2)}=\vec{F}_\alpha^{(1)}\otimes\vec{F}_\beta^{(1)}\,,\quad \alpha,\ \beta=1,\ldots,6 \tag{3.9}$$

with the corresponding eigenvalues

$$\lambda_{\alpha\beta}^{(2)}=\lambda_\alpha^{(1)}+\lambda_\beta^{(2)}\,,\quad \alpha,\ \beta=1,\ldots,6\,. \tag{3.10}$$

We note here that the eigenvectors $\vec{F}_{\beta\alpha}^{(2)}=\vec{F}_\beta^{(1)}\otimes\vec{F}_\alpha^{(1)}$ and $\vec{F}_{\alpha\beta}^{(2)}$ are different vectors although they are eigenvectors corresponding to the same eigenvalue $\lambda_{\alpha\beta}^{(2)}=\lambda_\alpha^{(1)}+\lambda_\beta^{(2)}$; this indicates that $\lambda_{\alpha\beta}^{(2)}$ $(\alpha\neq\beta)$ is an eigenvalue of at least double degeneracy.

We consider next the choice of appropriate linear combinations of solutions of the form of Eq. (3.5) to satisfy prescribed initial values $\langle X_k\rangle_0$ and $\langle \hat{X}_k\hat{X}_l\rangle_0$. That is, we wish to determine $c_\alpha^{(1)}$ and $c_{\alpha\beta}^{(2)}$ so that

$$\langle X_k\rangle_0=\sum_\alpha F_{k\alpha}^{(1)}c_\alpha^{(1)}\,,\quad \langle \hat{X}_k\hat{X}_l\rangle_0=\sum_{\alpha,\beta}F_{kl,\alpha\beta}^{(2)}c_{\alpha\beta}^{(2)}\,, \tag{3.11}$$

where $F_{k\alpha}^{(1)}$ are the components of $\vec{F}_\alpha^{(1)}$, etc. This procedure is also facilitated by the tensor-product relation Eq. (3.9). Let $\underline{\mathcal{F}}_{(1)}$ be the 6×6 matrix whose α column is $\vec{F}_\alpha^{(1)}$ and $\underline{\mathcal{F}}_{(2)}$ be the 36×36 matrix whose $\alpha\beta$ column is $\vec{F}_{\alpha\beta}^{(2)}$. Then Eqs. (3.11) can be rewritten

$$\langle\vec{X}\rangle_0=\underline{\mathcal{F}}_{(1)}\vec{c}_{(1)}\,,\quad \langle\vec{\hat{X}}\vec{\hat{X}}\rangle_0=\underline{\mathcal{F}}_{(2)}\vec{c}_{(2)}\,, \tag{3.11'}$$

with solutions

$$\vec{c}_{(1)}=\underline{\mathcal{F}}_{(1)}^{-1}\langle\vec{X}\rangle_0\,,\quad \vec{c}_{(2)}=\underline{\mathcal{F}}_{(2)}^{-1}\langle\vec{\hat{X}}\vec{\hat{X}}\rangle_0\,. \tag{3.12}$$

Furthermore, from Eq. (3.9)

$$\underline{\mathcal{F}}_{(2)}=\underline{\mathcal{F}}_{(1)}\otimes\underline{\mathcal{F}}_{(1)}\,, \tag{3.13}$$

so that

$$\underline{\mathcal{F}}_{(2)}^{-1}=\underline{\mathcal{F}}_{(1)}^{-1}\otimes\underline{\mathcal{F}}_{(1)}^{-1}\,, \tag{3.14}$$

where the tensor-product notation for matrices in Eqs. (3.13) and (3.14) indicates the Kronecker product.[14] It is only necessary, therefore, to determine the inverse of $\underline{\mathcal{F}}_{(1)}$ directly; the inverse of $\underline{\mathcal{F}}_{(2)}$ can then be expressed explicitly in terms of $\underline{\mathcal{F}}_{(1)}^{-1}$ through Eq. (3.14).

The final solutions for the first- and second-order means then take the forms

$$\begin{aligned}\langle X_k\rangle(t)&=\sum_{\alpha=1}^{6}c_\alpha^{(1)}F_{k\alpha}^{(1)}e^{\lambda_\alpha^{(1)}t}\,,\\ \langle\hat{X}_k\hat{X}_l\rangle(t)&=\sum_{\alpha,\beta=1}^{6}c_{\alpha\beta}^{(2)}F_{kl,\alpha\beta}^{(2)}e^{\lambda_{\alpha\beta}^{(2)}t}\,.\end{aligned} \tag{3.15}$$

IV. TWO-DIMENSIONAL MOTION

For the purposes of this section it is convenient to take the coordinate axes q_1, q_2, q_3 in the principal directions of the quadratic form $V(\vec{q})$. We then specialize the general results developed thus far to the case in which $\vec{B}$ is directed in the q_3 direction, confine attention to the two-dimensional motion of the wave packet in the q_1, q_2 plane, and carry through the details of the calculation explicitly for this case. The matrix $\underline{C}$ [Eq. (3.2)] then takes the form

$$\underline{C}=\begin{pmatrix}0&0&1&0\\0&0&0&1\\-V_1&0&0&B\\0&-V_2&-B&0\end{pmatrix}\,, \tag{4.1}$$

where $V(\vec{q})=\frac{1}{2}(V_1q_1^2+V_2q_2^2)$ and B is the magnitude of $\vec{B}$. The four eigenvalues $\lambda^{(1)}$ of $\underline{C}$ are

$$\lambda^{(1)}=+\lambda,\ -\lambda,\ +\mu,\ -\mu\,, \tag{4.2}$$

where

$$\lambda=[\tfrac{1}{2}(a+b)]^{1/2}\,,\qquad \mu=[\tfrac{1}{2}(a-b)]^{1/2}\,, \tag{4.2'}$$

with

$$a=-(V_1+V_2+B^2)\,,\quad b=(a^2-4V_1V_2)^{1/2}\,. \tag{4.2''}$$

The matrix $\underline{\mathcal{F}}_{(1)}$ of corresponding eigenvectors is

$$\underline{\mathcal{F}}_{(1)}=\begin{pmatrix}\lambda^2+V_2&\lambda^2+V_2&B\mu&-B\mu\\-B\lambda&B\lambda&\mu^2+V_1&\mu^2+V_1\\\lambda(\lambda^2+V_2)&-\lambda(\lambda^2+V_2)&B\mu^2&B\mu^2\\-B\lambda^2&-B\lambda^2&\mu(\mu^2+V_1)&-\mu(\mu^2+V_1)\end{pmatrix}\,. \tag{4.3}$$

Its inverse $\underline{\mathcal{F}}_{(1)}^{-1}$ is

$$\underline{\mathcal{F}}_{(1)}^{-1}=\frac{1}{\Delta}\begin{pmatrix} -\lambda\mu(V_1+\mu^2)(\alpha+B^2\mu^2) & B\mu^3(\alpha+B^2\lambda^2) & -\mu(V_1+\mu^2)(\alpha+B^2\lambda^2) & B\lambda\mu(\alpha+B^2\mu^2) \\ -\lambda\mu(V_1+\mu^2)(\alpha+B^2\mu^2) & -B\mu^3(\alpha+B^2\lambda^2) & \mu(V_1+\mu^2)(\alpha+B^2\lambda^2) & B\lambda\mu(\alpha+B^2\mu^2) \\ -B\lambda^3(\alpha+B^2\mu^2) & -\mu\lambda(V_2+\lambda^2)(\alpha+B^2\lambda^2) & -B\lambda\mu(\alpha+B^2\lambda^2) & -\lambda(V_2+\lambda^2)(\alpha+B^2\mu^2) \\ B\lambda^3(\alpha+B^2\mu^2) & -\mu\lambda(V_2+\lambda^2)(\alpha+B^2\lambda^2) & -B\lambda\mu(\alpha+B^2\lambda^2) & \lambda(V_2+\lambda^2)(\alpha+B^2\mu^2) \end{pmatrix}, \tag{4.4}$$

where $\alpha=(V_1+\mu^2)(V_2+\lambda^2)$ and $\Delta=-2\lambda\mu(\alpha+B^2\lambda^2)\times(\alpha+B^2\mu^2)$.

With this determination of $\underline{\mathcal{F}}_{(1)}^{-1}$ the problem of the first-order means is completed; the explicit solution for a given set of initial conditions may be found by application of Eqs. (3.12) and (3.15). Since the behavior of the first-order means follows the classical motion, we do not consider them further here but turn to the second-order means.

In order to obtain the solutions for the second-order means, it is necessary to form the Kronecker product[14] of the matrix $\underline{\mathcal{F}}_{(1)}^{-1}$ with itself yielding $\underline{\mathcal{F}}_{(2)}^{-1}$, and then, for given initial conditions,[15] to use the second line of Eqs. (3.12) and (3.15).

For the special case in which $V_1=V_2=V>0$, i.e., an isotropic potential well with isotropic initial conditions for the wave packet, namely,

$$\langle\hat{q}_i\hat{q}_j\rangle_0=\delta_{ij}\chi_0,\quad \langle\hat{\pi}_i\hat{\pi}_j\rangle_0=\delta_{ij}\Omega_0 \tag{4.5}$$

with real parts of $\langle q_i p_j\rangle=\langle p_j q_i\rangle=0$, the resulting solutions for

$$\langle\hat{q}_1\hat{q}_1\rangle(t)=\langle\hat{q}_2\hat{q}_2\rangle(t)=\chi(t)$$

and for

$$\langle\hat{\pi}_1\hat{\pi}_1\rangle(t)=\langle\hat{\pi}_2\hat{\pi}_2\rangle(t)=\Omega(t)$$

take particularly simple forms

$$\chi(t)=\{[(2V+B^2)\chi_0-2\Omega_0]\cos(\lambda'+\mu')t + 2(V\chi_0+\Omega_0)\}(4V+B^2)^{-1}, \tag{4.6}$$

$$\Omega(t)=\{[2\Omega_0-(2V+B^2)\chi_0]V\cos(\lambda'+\mu')t + (V\chi_0+\Omega_0)(2V+B^2)\}(4V+B^2)^{-1},$$

where

$$\lambda'=-i\lambda=-i\left\{\tfrac{1}{2}\left[-(2V+B^2)+B(4V+B^2)^{1/2}\right]\right\}^{1/2};$$

$$\mu'=-i\mu=-i\left\{\tfrac{1}{2}\left[-(2V+B^2)-B(4V+B^2)^{1/2}\right]\right\}. \tag{4.7}$$

The off-diagonal second-order means $\langle\hat{q}_1\hat{q}_2\rangle$ and $\langle\hat{\pi}_1\hat{\pi}_2\rangle$, initially zero, remain so.

For the general case of anisotropic potential and anisotropic intial conditions, determination of the explicit form of the solution becomes very cumbersome, and we have not carried it through for arbitrary B. Rather we have restricted attention to the case in which B is small compared to V_1 and V_2 and $|V_1-V_2|$ and have considered the first-order corrections to the zero magnetic field case. For definiteness, we take $V_1<0$ and $V_2>0$, so that we have the case of wave-packet motion on a saddle point; the changes involved for the other cases will be apparent.

The expansion starts by writing $\underline{\mathcal{F}}_{(1)}$ [Eq. (4.3)] in the form

$$\underline{\mathcal{F}}_{(1)}=\underline{\mathcal{F}}_{(1)}^{0}+B\underline{\mathcal{F}}_{(1)}^{1}+O(B^2), \tag{4.8}$$

where

$$\underline{\mathcal{F}}_{(1)}^{0}=\begin{pmatrix} V_2-V_1 & V_2-V_1 & 0 & 0 \\ 0 & 0 & -(V_2-V_1) & -(V_2-V_1) \\ |V_1|^{1/2}(V_2-V_1) & -|V_1|^{1/2}(V_2-V_1) & 0 & 0 \\ 0 & 0 & -iV_2^{1/2}(V_2-V_1) & iV_2^{1/2}(V_2-V_1) \end{pmatrix} \tag{4.9}$$

and

$$\underline{\mathcal{F}}_{(1)}^{1}=\begin{pmatrix} 0 & 0 & iV_2^{1/2} & -iV_2^{1/2} \\ -|V_1|^{1/2} & |V_1|^{1/2} & 0 & 0 \\ 0 & 0 & -V_2 & -V_2 \\ V_1 & V_1 & 0 & 0 \end{pmatrix}. \tag{4.10}$$

In obtaining this expansion of $\mathcal{F}_{(1)}$, we have used the expansions of the eigenvalues λ and μ,

$$\lambda=|V_1|^{1/2}+O(B^2),\quad \mu=iV_2^{1/2}+O(B^2). \tag{4.11}$$

The remainder of the calculation utilizes this first-order form of $\mathcal{F}_{(1)}$ in the general procedure outlined above. We present only the first-order results for $\langle\hat{q}_i\hat{q}_j\rangle(t)=\chi_{ij}(t)$, $i,j=1,2$, since these are sufficient[3] to describe the tunneling behavior of such wave packets; solutions for $\langle\hat{\pi}_i\hat{\pi}_j\rangle(t)=\Omega_{ij}(t)$ may be obtained in the same fashion:

$$\chi_{11}(t)=\chi_{11}^0\cosh^2\lambda t-\frac{\Omega_{11}^0}{V_1}\sinh^2\lambda t+B\left[\left(\frac{|V_1|^{1/2}(V_1+V_2)\chi_{12}^0-2|V_1|^{1/2}\Omega_{12}^0}{V_1(V_2-V_1)}\right)\sinh\lambda t\cosh\lambda t\right.$$
$$\left.+\frac{2V_2^{1/2}}{V_2-V_1}\chi_{12}^0\sin\mu' t\cosh\lambda t+\frac{2|V_1|^{1/2}}{V_1(V_2-V_1)}\Omega_{12}^0\cos\mu' t\sinh\lambda t\right], \quad (4.12)$$

$$\chi_{12}(t)=\chi_{12}^0\cos\mu' t\cosh\lambda t+(-V_1V_2)^{-1/2}\Omega_{12}^0\sin\mu' t\sinh\lambda t$$
$$-B\left[\tfrac{1}{2}V_2^{-1/2}[(V_1+V_2)\chi_{11}^0-2\Omega_{22}^0]\sin\mu' t\cosh\lambda t+\tfrac{1}{2}|V_1|^{-1/2}[(V_1+V_2)\chi_{22}^0-2\Omega_{11}^0]\cos\mu' t\sinh\lambda t\right.$$
$$\left.+|V_1|^{1/2}\left(\chi_{11}^0-\frac{\Omega_{11}^0}{V_1}\right)\sinh\lambda t\cosh\lambda t-V_2^{1/2}\left(\chi_{22}^0-\frac{\Omega_{22}^0}{V_2}\right)\sin\mu' t\cos\mu' t\right](V_2-V_1)^{-1}, \quad (4.13)$$

$$\chi_{22}(t)=\chi_{22}^0\cos^2\mu' t+(\Omega_{22}^0/V_2)\sin^2\mu' t-B\{V_2^{-1/2}[(V_1+V_2)\chi_{12}^0-2\Omega_{12}^0]\sin\mu' t\cos\mu' t$$
$$+2|V_1|^{1/2}\chi_{12}^0\cos\mu' t\sinh\lambda t+2V_2^{-1/2}\Omega_{12}^0\sin\mu' t\cosh\lambda t\}(V_2-V_1)^{-1}. \quad (4.14)$$

In the derivation of these solutions, the initial conditions were chosen to correspond to the case in which the initial value of a_{ij} [Eq. (2.4)] was taken as zero.

As outlined in Weiner and Partom,[3] the probability $P(t)$ of finding the particle within the region $q_1>0$, i.e., beyond the crest of the saddle point, is given by

$$P(t)=\tfrac{1}{2}\operatorname{erfc}[-\langle q_1\rangle(t)/(2\chi_{11})^{1/2}]. \quad (4.15)$$

For the present case the mean motion $\langle q_1\rangle(t)$ is found to be

$$\langle q_1\rangle(t)=\langle q_1\rangle_0\cosh\lambda t+|V_1|^{-1/2}\langle\pi_1\rangle_0\sinh\lambda t$$
$$+B(V_2-V_1)^{-1}(\langle\pi_2\rangle_0\cosh\lambda t-V_2|V_1|^{-1/2}\langle q_2\rangle_0\sinh\lambda t$$
$$+V_2^{1/2}\langle q_2\rangle_0\sin\mu' t-\langle\pi_2\rangle_0\cos\mu' t). \quad (4.16)$$

V. PARTICLE-METHOD CALCULATIONS

A procedure, termed the particle method, for the solution of the time-dependent Schrödinger equation has been described[2,12] for the case of zero magnetic field. This method is based on the hydrodynamic analogy to the Schrödinger equation. The original form of this analogy[16] is readily extended to include magnetic fields,[17] and it is correspondingly straightforward to extend the particle method as well to this case. In this section we briefly describe this extension, give two examples of computations utilizing this method, and compare the results with the analytical solutions of Sec. IV. In both of the numerical examples we have chosen the values of the parameters arbitrarily, simply in order to demonstrate the qualitative behavior of the solutions; we have not attempted to select values characteristic of a given physical situation.

To derive the hydrodynamic analogy in the presence of a magnetic field we substitute the wave function ψ expressed in terms of its amplitude R and S [Eq. (2.3)] into the Schrödinger equation [Eq. (2.1)] and equate real and imaginary parts with the results

$$\frac{\partial S}{\partial t}+\tfrac{1}{2}(\nabla S-\vec{A})^2+V-\frac{1}{2}\frac{\nabla^2 R}{R}=0, \quad (5.1)$$

$$\frac{\partial R^2}{\partial t}+\nabla\cdot[R^2(\nabla S-\vec{A})]=0. \quad (5.2)$$

We take the gradient of Eq. (5.1) and introduce the following notation:

$$\vec{v}(\vec{q},t)=\nabla S-\vec{A},$$
$$V_{qu}(\vec{q},t)=-\tfrac{1}{2}\nabla^2 R/R, \quad (5.3)$$
$$\rho(\vec{q},t)=R^2.$$

Then Eqs. (5.1) and (5.2) become

$$\frac{dv}{dt}=-\nabla V+\vec{v}\times\vec{B}-\nabla V_{qu}, \quad (5.4)$$

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\vec{v})=0, \quad (5.5)$$

where

$$\frac{d\vec{v}}{dt}=\frac{\partial\vec{v}}{\partial t}+\vec{v}\cdot\nabla\vec{v}. \quad (5.6)$$

From these equations the hydrodynamic analogy in the presence of a magnetic field follows. They indicate that the time evolution of the wave function $\psi(\vec{q},t)$ is equivalent to the flow of a fluid of density $\rho(\vec{q},t)$ whose particles, moving with velocity $\vec{v}(\vec{q},t)$, are subject to a force derived from the prescribed potential $V(\vec{q})$, a Lorentz force[18] $\vec{v}\times\vec{B}$, plus an additional force derived from the "quantum potential" $V_{qu}(\vec{q},t)$ which depends upon the fluid density as in Eq. (5.3). Equation (5.4) will be recognized as the equation of motion and Eq. (5.5) as the equation of continuity for such a continuum, while Eq. (5.6) is the equation for the particle acceleration when

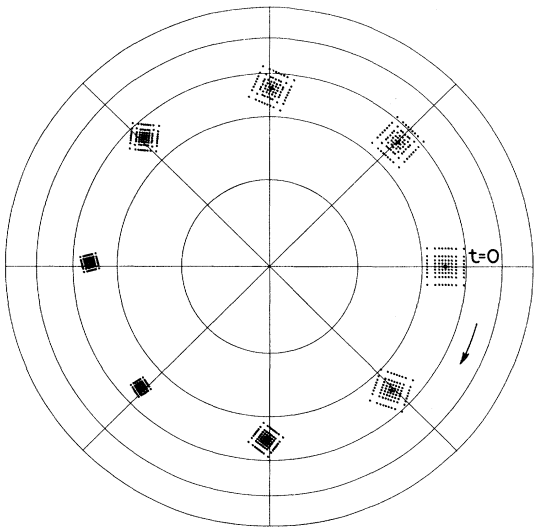

FIG. 1. Isotropic Gaussian wave packet representing electron in isotropic potential well with magnetic field vector pointing into paper. Figure shows a representative set of "particles" (from the viewpoint of the hydrodynamic analogy) at successive times along the wave-packet trajectory. Note that the wave packet "spins" and its radius pulsates as its mean follows the classical trajectory. The magnetic field is $B=+2$ (pointing into paper). Wave-packet dimensions are shown in one-half scale for figure clarity.

Eulerian coordinates are employed to designate particle position.

In the particle method for the solution of the time-dependent Schrödinger equation, the fluid is approximated by a finite collection of representative particles and their trajectories are calculated by the numerical solution of Eqs. (5.4) and (5.5). Details for the zero magnetic field case may be found in the paper by Weiner and Askar[12]; as seen from Eq. (5.4) the only modification needed here is the addition of the Lorentz force in computing the trajectory of each representative particle of the continuum.

We consider first the results of a numerical computation using the particle method for the problem of an isotropic potential well with isotropic initial conditions for which a compact expression of the exact solution, Eq. (4.6), is available. The following dimensionless parameters were selected arbitrarily:

$$V_1 = V_2 = 1 ;$$

$$\langle q_1\rangle_0 = 8.0 , \quad \langle q_2\rangle_0 = 0 ,$$

$$\langle \pi_1\rangle_0 = 0 , \quad \langle \pi_2\rangle_0 = -19.314 .$$

The value of $\langle \pi_2\rangle_0$ was chosen according to the formula

$$\langle \pi_2\rangle_0 = -\tfrac{1}{2}\langle q_1\rangle_0 [B + (4V + B^2)^{1/2}]$$

so as to give rise to a closed circular orbit:

$$\langle \hat{q}_1\hat{q}_1\rangle_0 = \langle \hat{q}_2\hat{q}_2\rangle_0 = 1 , \quad \langle \hat{q}_1\hat{q}_2\rangle_0 = \langle \hat{p}_1\hat{p}_2\rangle_0 = 0 ,$$

$$\langle \hat{q}_i\hat{p}_j\rangle_0 = \langle \hat{p}_j\hat{q}_i\rangle_0 = 0 , \quad \langle \hat{p}_1\hat{p}_1\rangle_0 = \langle \hat{p}_2\hat{p}_2\rangle_0 = \tfrac{1}{4} ;$$

$$B = +2 .$$

The large magnitude of B was used so that the qualitative features of the solution are readily apparent.

Although the wave packet is isotropic, a square array of 9×9 representative particles was chosen for the computation with the density of the initial array chosen to correspond to $R^2(\vec{q}, 0)$. The use of a square array is computationally convenient and also makes the results of the computation easier to visualize. The particle "velocity" $\vec{v}$ [Eq. (5.3)] for a Gaussian wave packet [Eqs. (2.3) and (2.4)] in a uniform magnetic field takes the following simple form:

$$v_i(\vec{q}, t) = \langle \pi_i\rangle(t) + a_{ij}(t)\,\hat{q}_j - A_{ij}\,\hat{q}_j . \tag{5.7}$$

That is, superimposed on the mean motion $\langle \pi_i\rangle(t)$ which obeys the classical equations is a stretching motion due to the symmetric matrix $a_{ij}(t)$ and a spin due to the antisymmetric A_{ij}. A computer-plotted (Calcomp system) result of the particle-method computations is shown in Fig. 1; in it may be seen both the "spin" of the wave packet and its expansion and contraction.

We present next the results of a sample problem chosen to illustrate the effects of a magnetic field on the dynamics of a Gaussian wave packet on a quadratic saddle point with particular emphasis on the magnetic field effect upon the tunneling through such a barrier. The dimensionless parameters of the sample problem were chosen arbitrarily as follows:

$$V_1 = -1 , \quad V_2 = +1$$

so that the equation of the saddle-point surface is

$$V(q_1, q_2) = \tfrac{1}{2}(-q_1^2 + q_2^2) ;$$

$$\langle q_1\rangle_0 = -3.0 , \quad \langle q_2\rangle_0 = +3.0 ,$$

$$\langle \pi_1\rangle_0 = 2.0 , \quad \langle \pi_2\rangle_0 = -15.0 .$$

In classical terms, therefore, the potential-energy barrier which the wave packet must overcome has a magnitude of 4.5 a.u., and the kinetic energy of its motion in the $\hat{q}_1$ direction is 2 a.u.:

$$\langle \hat{q}_1\hat{q}_1\rangle_0 = 0.5 , \quad \langle \hat{q}_2\hat{q}_2\rangle_0 = 0.3 , \quad \langle \hat{q}_1\hat{q}_2\rangle_0 = 0.15 ,$$

$$\langle \hat{q}_i\hat{p}_j\rangle_0 = \langle \hat{p}_j\hat{q}_i\rangle_0 = 0 , \quad \langle \hat{p}_i\hat{p}_j\rangle_0 = \tfrac{1}{4}\langle \hat{q}_i\hat{q}_j\rangle_0^{-1} .$$

Here the notation $\langle \hat{q}_i\hat{q}_j\rangle_0^{-1}$ refers to the matrix inverse. It may be verified for a Gaussian wave packet, Eqs. (2.3) and (2.4), that this choice for

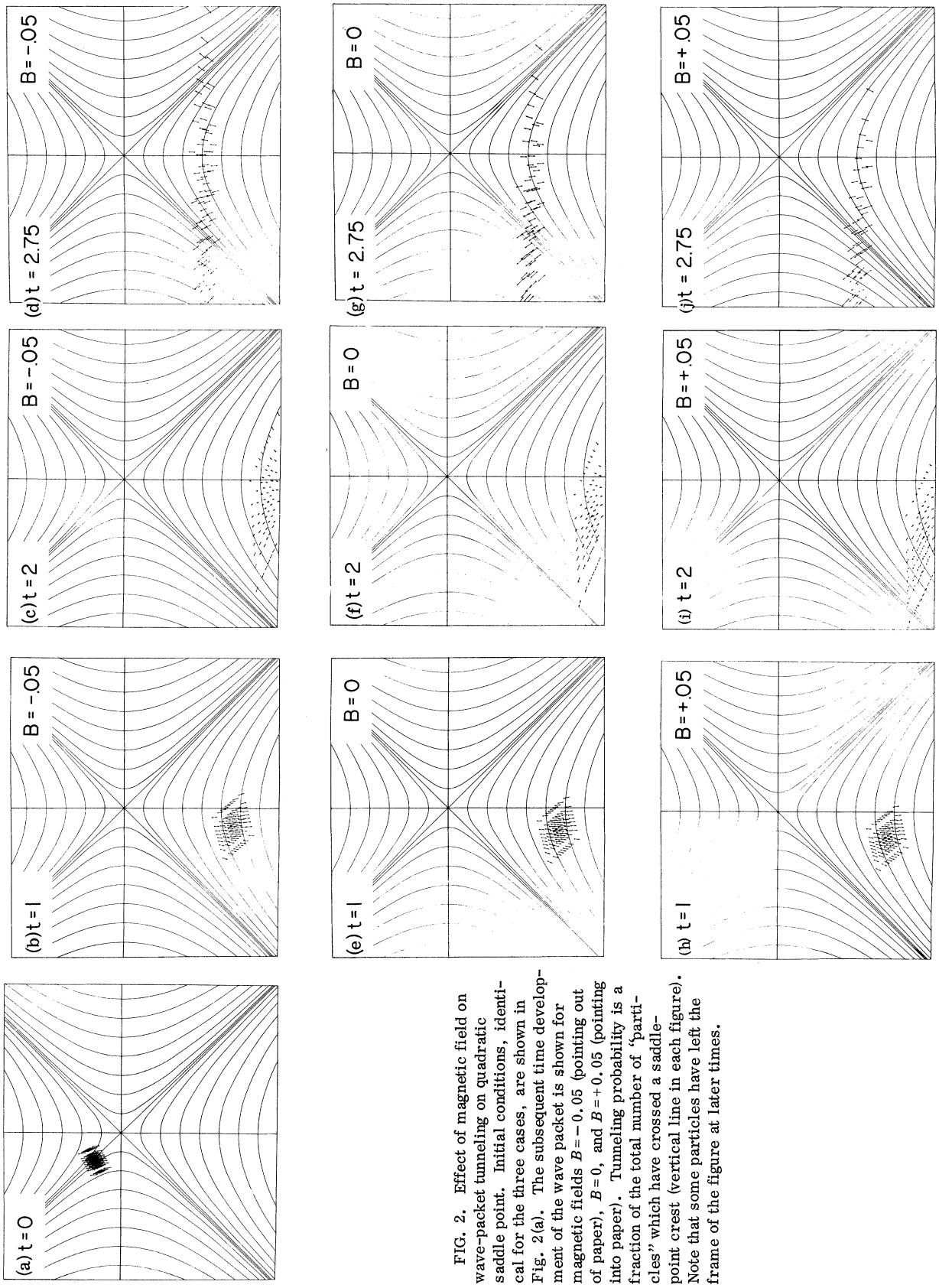

FIG. 2. Effect of magnetic field on wave-packet tunneling on quadratic saddle point. Initial conditions, identical for the three cases, are shown in Fig. 2(a). The subsequent time development of the wave packet is shown for magnetic fields $B=-0.05$ (pointing out of paper), $B=0$, and $B=+0.05$ (pointing into paper). Tunneling probability is a fraction of the total number of "particles" which have crossed a saddle-point crest (vertical line in each figure). Note that some particles have left the frame of the figure at later times.

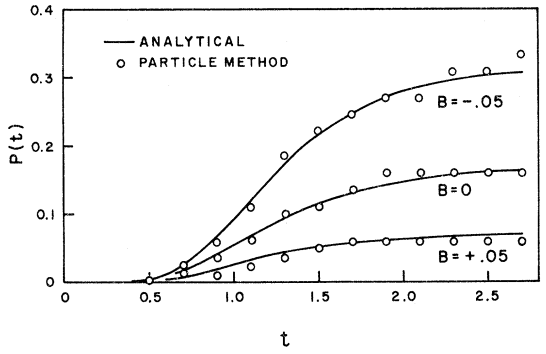

FIG. 3. Comparison of time-dependent-tunneling probability $P(t)$ as given by the analytical solution and by the numerical solution using the particle method. Units in which $m=\hbar=1$ are employed.

$\langle \hat{p}_i \hat{p}_j \rangle_0$ corresponds to the case of $a_{ij}(0)$, Eq. (2.4), equal to zero.

The magnetic field was taken as in Sec. IV, in the q_3 direction; three values of the component B in this direction were considered, namely,

$$B=0\ ,\ \pm 0.05\ .$$

A rectangular array of 9×9 particles was again employed in the particle-method computation. This initial array is shown in Fig. 2(a) which also shows the velocities of the particles corresponding to the initial conditions listed above. The other figures show the subsequent wave-packet dynamics. In general it may be noted that in the wave-packet motion, the wave-packet width in the q_2 direction (the direction of positive curvature of the saddle point) remains fairly constant, and the wave packet oscillates back and forth in this direction with a reversal in this sequence of figures taking place between $t=1$ and $t=2$. On the other hand, the wave-packet width in the q_1 direction (the direction of negative curvature of the saddle point) grows exponentially and gives rise to the tunneling across the barrier as evidenced by the crossing of the saddle-point (the vertical line in each figure) by some of the representative particles of the packet; the tunneling probability at any time is given by the fraction of the total number of particles employed which have crossed the crest. The influence of the magnetic field upon the tunneling may be seen in the final time step of these figures, $t=2.75$. The value of $B=0.05$ was chosen to be sufficiently large to make this influence marked. If the mass of the electron is employed, this value of B corresponds to a field strength of 1.2×10^6 G; clearly this effect could only become important at attainable field strengths for processes in which a greatly reduced effective electronic mass was appropriate.[19]

A comparison of the results of the particle-method calculation and the analytical solution of Sec. IV correct to first order in B reveals good agreement. As an example, the tunneling probability at time t, $P(t)$, is shown in Fig. 3 as determined by both methods. Some of the discrepancy between the analytical and particle method results from the fact that in the latter the tunneling probability can only change by discrete jumps ($\frac{1}{81}$) whenever a representative particle crosses the crest.

VI. CONCLUDING REMARKS

This paper has presented the treatment of Gaussian wave-packet dynamics in a uniform magnetic and quadratic potential field, based on the ordinary differential equations satisfied by the first- and second-order quantum means. Our principal result is the development of a tensor-product relationship of the second- to first-order problem which greatly simplifies the calculations.

Two particular problems have been treated in detail. In the first the quadratic potential represents an isotropic potential well. With the additional restriction to the case of an isotropic wave packet, the solution may be obtained in compact closed form. The second problem treats the case of a wave packet on a saddle point. Here the principal interest is the effect of a magnetic field upon the tunneling through such a barrier, and the explicit solution is obtained only to first order in the field strength. This problem was suggested by a theory of rate processes in solids[1-3] in which a system in a trapped localized state in thermal equilibrium is represented by a suitable ensemble of Gaussian wave packets. The present calculation indicates that magnetic field effects on the escape of trapped localized electrons should be very small at presently attainable field strengths unless the effective electronic mass is greatly reduced.

The two problems just described have also been treated here numerically by a technique referred to as the particle method[2,12] which is based on the hydrodynamic analogy to the time-dependent Schrödinger equation. The numerical results agree well with the analytical solutions and suggest that this method may be useful for examining wave-packet dynamics for cases in which analytical solutions are not possible. However, it should be emphasized that Gaussian-wave-packet dynamics under the conditions considered here present a case which is particularly simple from the viewpoint of the hydrodynamic analogy because the velocity field is linear [Eq. (5.7)]. Current work here on more complex flows have revealed serious difficulties which must be overcome before the particle method can be applied to them.

*Research supported by National Science Foundation Grant No. GJ-30105.

†Present address: Department of Mathematics, University of Michigan, Ann Arbor, Michigan.

[1]J. H. Weiner, Phys. Rev. 169, 570 (1968).

[2]J. H. Weiner and Y. Partom, Phys. Rev. 187, 1134 (1969).

[3]This procedure has also been used in the zero magnetic field case by J. H. Weiner and Y. Partom, Phys. Rev. B 1, 1533 (1970).

[4]See, for example, the recent paper by G. E. Pike, Phys. Rev. B 6, 1572 (1972), and the references contained therein.

[5]C. G. Darwin, Proc. Camb. Phil. Soc. 27, 86 (1930). The energy eigenvalues and eigenfunctions for this problem were found earlier by V. Fock, Z. Physick 47, 446 (1928).

[6]K. Husimi, Prog. Theoret. Phys. (Kyoto) 9, 238 (1953).

[7]I. A. Malkin and V. I. Man'ko, Zh. Eksp. Teor. Fiz. 59, 1746 (1970) [Sov. Phys.-JETP 32, 949 (1971)].

[8]A. Feldman and A. H. Kahn, Phys. Rev. B 1, 4584 (1970).

[9]W. G. Tam, Physica 54, 557 (1971).

[10]G. J. Papadopoulos, J. Phys. A 4, 773 (1971).

[11]D. Langbein, Phys. Kondens Materie 10, 21 (1969); 10, 29 (1969); 10, 44 (1969). [*Note added in proof.* See also the recent papers by D. H. Thomson, Am. J. Phys. 40, 1669 (1972); Am. J. Phys. 40, 1673 (1972), which deal with the effect of the choice of electromagnetic gauge.]

[12]J. H. Weiner and A. Askar, J. Chem. Phys. 54, 3534 (1971).

[13]We include in the definition of Gaussian as used here the fact that the phase of ψ is quadratic in the coordinates, as in Eq. (2.4).

[14]For the notation and concepts used here we refer to P. R. Halmos, in *Finite-Dimensional Vector Spaces*, 2nd ed. (Van Nostrand, New York, 1958), pp. 38–41, 95–98. In particular when we wish to transcribe linear transformations and vectors in the tensor product space as matrices and column vectors, respectively, we use lexicographical ordering as described on p. 97 of this reference.

[15]It should be noted that the quantities $\langle \hat{q}_i \hat{\pi}_j \rangle$ and $\langle \hat{\pi}_i \hat{\pi}_j \rangle$ have nonzero constant imaginary parts which identically satisfy the differential equations (2.14). Since only the real quantities $\langle \hat{q}_i \hat{\pi}_j \rangle + \langle \hat{\pi}_j \hat{q}_i \rangle$ and $\langle \hat{\pi}_i \hat{\pi}_j \rangle + \langle \hat{\pi}_j \hat{\pi}_i \rangle$ are of interest, only the real parts of the initial values of $\langle \hat{q}_i \hat{\pi}_j \rangle$ and $\langle \hat{\pi}_i \hat{\pi}_j \rangle$ need be considered.

[16]E. Madelung, Z. Physik 40, 322 (1926); L. de Broglie, Compt. Rend. 183, 447 (1926). For a recent discussion and further references see H. E. Wilhelm, Phys. Rev. D 1, 2278 (1970).

[17]T. Takabayasi, Prog. Theoret. Phys. (Kyoto) 8, 143 (1952).

[18]By employing atomic units in which the magnitude of the electronic charge $e=1$, we have lost an indicator of the sign of the charge under discussion. We adopt the convention, therefore, that when the charge is negative, as is the case for all the numerical (two-dimensional) examples here considered, the positive direction of B is the negative q_3 direction (q_1, q_2, q_3 a right-handed system).

[19]B. B. Suprapto and A. K. Das, Phys. Status Solidi B 50, 253 (1972).

PHYSICAL REVIEW B VOLUME 7, NUMBER 4 15 FEBRUARY 1973

Lattice Dynamical Study of Indium*

B. Sharan

Department of Science Education, National Council of Educational Research and Training, New Delhi-16, India

and

Ashok Kumar

Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi-29, India

(Received 2 May 1972)

The lattice dynamics of the body-centered tetragonal crystal has been investigated. The interatomic forces considered include, in addition to the central forces and angular forces of the type employed by Clark, Gazis, and Wallis, those forces arising from certain energies owing to the compressibility of the conduction electrons and their interaction with ions. The approach has been utilized to study the metal indium, and results are presented for the dispersion curves and the Debye temperature.

INTRODUCTION

The Debye temperature and dispersion curves have been studied for the body-centered tetragonal indium. The interatomic forces used consist of central, angular, and volume forces. The angular forces have been incorporated in a manner suggested by Clark, Gazis, and Wallis.[1] The volume forces, owing their origin to free conduction electrons, have been considered in a semiphenomenological way, viz., by averaging the effect of the presence of electrons on lattice vibrations over the actual shape of the Wigner–Seitz polyhedron.

The chief aim of the investigation is to give a