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Wave function for harmonically confined electrons in time-dependent electric and magnetostatic fields

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We derive via the interaction "representation" the many-body wave function for harmonically confined electrons in the presence of a magnetostatic field and perturbed by a spatially homogeneous time-dependent electric field—the Generalized Kohn Theorem (GKT) wave function. In the absence of the harmonic confinement—the uniform electron gas—the GKT wave function reduces to the Kohn Theorem wave function. Without the magnetostatic field, the GKT wave function is the Harmonic Potential Theorem wave function. We further prove the validity of the connection between the GKT wave function derived and the system in an accelerated frame of reference. Finally, we provide examples of the application of the GKT wave function. © 2014 AIP Publishing LLC.

I. INTRODUCTION

A basic problem in quantum mechanics is the determination of the solution to the many-electron system in atoms, molecules, solids, quantum wells, two-dimensional electron systems such as those at semiconductor heterojunctions, quantum dots, etc., and of the interaction of such systems with external electromagnetic fields. Systems for which exact solutions of the Schrödinger equation exist are uncommon, and thus such systems play a significant role in the understanding of the many-body problem. The exact solutions also lead to further physical insights via their use in other manifestations of Schrödinger theory such as density functional1–6 and quantal density functional7, 8 theories. In this paper we consider a time-dependent (TD) Hamiltonian that is modifiable and hence applicable to different physical systems,9–13 and provide a first-principles derivation of the corresponding (most general) wave function which we refer to as the Generalized Kohn Theorem (GKT) wave function.

Consider a system of N harmonically confined electrons in a magnetostatic field $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$. On a spatially homogeneous time-dependent electric field $\mathbf{E}(t)$, the Hamiltonian is

$$\hat{H}(t) = \hat{H}(0) + e\mathbf{E}(t) \cdot \sum_i \mathbf{r}_i,$$

where the unperturbed Hamiltonian is

$$\hat{H}(0) = \sum_i \left[ \frac{1}{2m} \left( \hat{\mathbf{p}}_i + \frac{e}{c} \mathbf{A}(\mathbf{r}_i) \right)^2 + \frac{1}{2} \mathbf{r}_i \cdot \mathbf{\mathbb{K}} \cdot \mathbf{r}_i \right] + \sum_{(i,j)} u(\mathbf{r}_i - \mathbf{r}_j),$$

with $i = 1, \ldots, N$ denotes the electrons; $(i, j)$ denotes all pairs; $\mathbf{r}_i = (x_i, y_i, z_i); u(\mathbf{r})$ the electron interaction operator; and $\mathbb{K}$ is the force constant matrix

$$\mathbb{K} = m \begin{pmatrix} \omega_x^2 & 0 & 0 \\ 0 & \omega_y^2 & 0 \\ 0 & 0 & \omega_z^2 \end{pmatrix},$$

and $\omega_x, \omega_y, \omega_z$ the directional harmonic frequencies. The corresponding (most general) wave function which we refer to as the Generalized Kohn Theorem (GKT) wave function. In the symmetric gauge

$$\Psi_n(\mathbf{r}_1, \ldots, \mathbf{r}_N; t) = \tilde{\Psi}_n(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{R}_m(t), \mathbf{R}_m(t)) \times \tilde{\Psi}_m(\mathbf{r}_1 - \mathbf{R}_m(t), \mathbf{r}_2 - \mathbf{R}_m(t), \ldots, \mathbf{r}_N - \mathbf{R}_m(t)),$$

where $E_n, \tilde{\Psi}_n$ are the eigenenergies and eigenfunctions of the unperturbed Hamiltonian:

$$\hat{H}(0)\tilde{\Psi}_n(\mathbf{r}_1, \ldots, \mathbf{r}_N) = E_n\tilde{\Psi}_n(\mathbf{r}_1, \ldots, \mathbf{r}_N);$$

$S_0[\mathbf{R}_m(t)]$ the total classical action:

$$S_0[\mathbf{R}_m(t)] = S_0^{XY}(t) + S_0^Z(t),$$

$$S_0^{XY}[\mathbf{R}_m(t)] = \frac{1}{2} M \int_0^t \left( \mathbf{R}_m^2(t) - \mathbf{R}_m^2(t) \right) dt' + \omega_z \mathbf{R}_m \cdot \mathbf{J} \mathbf{R}_m dt',$$
\[
S_0^2[Z(t)] = \frac{1}{2} M \int_0^t \left( \dot{Z}^2 - \omega_c^2 Z^2 \right) dt'.
\] (9)

In Eq. (5), \( \mathbf{R}_m(t) \) is the three-dimensional vector \((X_m(t), Y_m(t), Z_m(t))\), and
\( \mathbf{R}_{p(t)} \) the corresponding canonical momentum (see Eq. (68) below). The vector \( \mathbf{R}_m(t) \) satisfies the classical equation of motion
\[
m \frac{d^2 \mathbf{R}_m(t)}{dt^2} = -\mathbf{H} - eE(t) \mathbf{R}_m(t) - \frac{e}{c} \frac{d \mathbf{R}_m(t)}{dt} \times \mathbf{B}. \tag{10}
\]

In Eq. (8), \( \mathbf{R}_s(t) \) is the two-dimensional vector \((X_s(t), Y_s(t))\); \( \mathbf{R}_s \) the transpose of the vector \( \mathbf{R}_s \); \( \Omega^2 = (\omega_x^2 \omega_y^2) \); and \( J = (0 1 0) \).

Finally, the vector in Eq. (5) \( \mathbf{R} = \frac{1}{N} \sum \mathbf{r}_i = \left( \frac{X}{Z} \right) \),
\[
\omega_c = \frac{NeB}{Mc} = \frac{eB}{mc} \text{ the cyclotron frequency, and } M = Nm.
\]

Observe that the GKT wave function is comprised of a phase factor times the unperturbed wave function in which the coordinates of each electron are translated by a value that satisfies the classical equation of motion. Hence, if the unperturbed wave function is known, then the time evolution of all properties is known. In particular, observables represented by non-differential Hermitian operators such as the density \( \rho(r, t) = \langle \Psi | \hat{\rho}(r) | \Psi \rangle \), with \( \hat{\rho}(r) = \sum \delta(\mathbf{r}_i - \mathbf{r}) \) the density operator, possess the translational property
\[
\rho(r, t) = \rho_0(r - \mathbf{R}_m(t)), \tag{11}
\]
where \( \rho_0(r) \) is the unperturbed system density. Thus, if the unperturbed wave function and hence density \( \rho_0(r) \) is known, then so is the time evolution of the perturbed system density \( \rho(r, t) \). Because of the phase factor this translational property is not obeyed for observables involving differential operators such as the physical current density. We note two special cases of the wave function: In the absence of the external harmonic potential, i.e., for the uniform electron gas, the GKT wave function derived reduces to the Kohn theorem (KT) wave function; in the absence of the external magnetic field, the GKT wave function reduces to that of the harmonic potential theorem (HPT) wave function. (For other independent derivations of the HPT wave function via the operator, Feynman Path integral, and interaction “representation” methods see, respectively, Refs. 7, 15, and 16.)

We next put our work in context. In the original work by Kohn and co-workers, it was shown that for systems represented by the Hamiltonian of Eq. (1), the optical absorption frequencies observed, whether for the uniform electron gas or when the electrons are confined harmonically, were identical to those of a single particle and independent of the number of electrons and the electron-electron interaction. (In the literature, the case of the uniform electron gas is considered the KT; and that of the harmonically confined electrons case is referred to as the GKT.) However, in spite of the fact that Yip states in his footnote 8 that “It is straightforward to deduce the ground-state wave function (and thus also the excited states)” the explicit expression for the GKT wave function of Eq. (5) is not given in these papers.

In a later paper, Dobson derived the HPT wave function stating that this was a “slight extension of the GKT” since “the GKT only refers to the frequency dependence of linear response and does not address the spatial profile of the moving density.” By “extension” Dobson was referring to the derivation of the HPT wave function. From the wave function it becomes clear that the density \( \rho(r, t) \) must satisfy the transversal property of Eq. (11). As the density \( \rho(r, t) \) is the basic ingredient of TD density functional theory, this property of the density could then be employed as a rigorous constraint to test various approximate action functionals of the density within the context of the theory.

Again, with the purpose of testing different action functionals, Vignale observed that the density \( \rho(r, t) \) corresponding to the GKT Hamiltonian of Eq. (1) also obeyed the translational property of Eq. (11). He arrived at this conclusion by considering the Schrödinger equation in an accelerated frame of reference. As the focus of TD density functional theory is the density \( \rho(r, t) \), neither the GKT wave function nor its derivation via this approach were provided. (The expression for the KT wave function now appears in the text of Ref. 19.)

Thus, the expression for the GKT wave function does not exist in the literature at present. Knowledge of the GKT wave function leads directly to the translational property of the density, and to the KT and HPT wave functions since these constitute special cases. It is evident that there are several approaches by which the wave function could be derived. For example, one could employ the operator method of Kohn and co-workers or of the accelerated frame of reference approach due to Vignale. Here we provide a first principles derivation via the interaction “representation” that differs from these methods. Further, in the Appendix we consider the Vignale approach, and prove the validity of the connection between the wave function derived and the Hamiltonian in the accelerated frame of reference. Finally, we provide examples of the application of the GKT wave function.

II. SEPARATION OF HAMILTONIAN

The key to the derivation of the GKT wave function, and of course to the understanding of the optical absorption frequencies, is that the Hamiltonian of Eq. (1) is separable into its center of mass and relative coordinate components. The center of mass component is that of a single particle of mass \( Nm \) and charge \( Ne \) confined harmonically by \( N \) times the potential of a single particle. The effect of the TD electric field also appears only in this component. The electron interaction potential term appears only in the relative coordinate component of the Hamiltonian. Furthermore, the in-plane center of mass motion component of the Hamiltonian is separable from the motion in the plane perpendicular to it which is the assumed direction of the magnetic field.

To see this, define the center of mass and relative coordinates and momenta as
\[
\mathbf{R} \equiv \mathbf{R}^{(1)} = \frac{1}{N} \sum \mathbf{r}_i; \quad \Pi \equiv \Pi^{(1)} = \sum \hat{\pi}_i;
\]
\[
\hat{\pi}_i = -i\hbar \nabla_i + \frac{e}{c} \mathbf{A} (\mathbf{r}_i),
\] (12)
and
\[ X^{(2)} = x_1 - x_2, \]
\[ X^{(3)} = x_1 + x_2 - 2x_3, \ldots, \]
\[ X^{(N)} = x_1 + x_2 + \ldots + x_{N-1} - (N-1)x_N, \tag{13} \]
and similarly for \( Y^{(2)}, \ldots, Y^{(N)}, Z^{(2)}, \ldots, Z^{(N)}, \) and \( \Pi^{(2)}, \ldots, \Pi^{(N)}. \)

The Hamiltonian can then be rewritten as
\[ \hat{H} = \hat{H}_{cm} + \hat{H}_{rel}, \tag{14} \]
where the center of mass Hamiltonian \( \hat{H}_{cm}(t) \) is
\[ \hat{H}_{cm}(t) = \frac{\Pi^2}{2M} + \frac{M}{2}(\omega_x^2 X^2 + \omega_y^2 Y^2 + \omega_z^2 Z^2) - NeE(t) \cdot R, \tag{15} \]
with
\[ \hat{N} = -i\hbar \nabla_R + \frac{Ne}{c} A(R), \tag{16} \]
and \( M = Nm. \) \( \hat{H}_{rel} \) is the Hamiltonian of the relative coordinates and contains the effects of the interaction. It can be readily shown that \( [\hat{H}_{cm}, \hat{H}_{rel}] = 0 \) so that the center-of-mass motion and the relative motion are separable. Therefore, the eigenstates of the Hamiltonian are the product of the eigenstates of the center-of-mass motion \( \Phi(R, t) \) and the relative motion \( \varphi_{rel}(R^{(2)}, \ldots, R^{(N)}): \)
\[ \psi(r_1, r_2, \ldots, r_N, t) = \Phi(R, t)\varphi_{rel}(R^{(2)}, \ldots, R^{(N)}). \tag{17} \]

The relative motion wave function \( \varphi_{rel}(R^{(2)}, \ldots, R^{(N)}) \) satisfies
\[ \hat{H}_{rel}\varphi_{rel}(R^{(2)}, \ldots, R^{(N)}) = E_{rel}\varphi_{rel}(R^{(2)}, \ldots, R^{(N)}), \tag{18} \]
where \( E_{rel} \) is the corresponding eigenvalue.

We next focus on the \( \hat{H}_{cm}(t) \) since the effect of the external electrical field appears only in the center-of-mass motion. For simplicity, choosing the direction of the magnetic field as the \( z \) direction, then in the symmetric gauge \( A(R) = (-\frac{By}{c}, \frac{Bx}{c}, 0) \), and Eq. (15) can be decomposed into two parts
\[ \hat{H}_{cm}(t) = \hat{H}_{XY}(t) + \hat{H}_{Z}(t), \tag{19} \]
where \( \hat{H}_{XY}(t) \) describes the in-plane motion, and
\[ \hat{H}_{Z}(t) = \frac{1}{2M} \hat{P}_Z^2 + \frac{1}{2} M\omega_z^2 Z^2 + NeE_z(t) Z, \tag{20} \]
describes a trivial motion in the \( Z \)-direction without the influence of the magnetic field. This motion is independent of the in-plane motion, and as such the center-of-mass wave function \( \Phi(R, t) \) is just the product of the in-plane motion wave function and the \( Z \)-direction wave function. The latter is simply the one-dimensional HPT wave function. For the expression of the in-plane relative coordinate Hamiltonian, see the supplementary material.\(^{21}\)

III. IN-PLANE CENTER-OF-MASS MOTION

We next focus on the in-plane motion described by \( \hat{H}_{XY}(t) \), which may be further separated as
\[ \hat{H}_{XY}(t) = \hat{H}_0 + \hat{H}_1(t), \tag{21} \]
where the time-independent part is
\[ \hat{H}_0 = \frac{1}{2M} (\hat{P}_X^2 + \hat{P}_Y^2) + \frac{1}{2} M(\omega_x^2 X^2 + \omega_y^2 Y^2), \]
\[ = \frac{1}{2M} (\hat{E}_x^2 + \hat{E}_y^2) + \frac{1}{2} M(\omega_x^2 X^2 + \omega_y^2 Y^2) + \frac{\omega_e}{2} \hat{L}_Z, \tag{22} \]
with \( \omega_1^2 = \omega_x^2 + \omega_y^2, \omega_2^2 = \omega_x^2 + \omega_z^2, \omega_e = \frac{NeE}{mc} \) is the cyclotron frequency, and \( \hat{L}_Z = X\hat{P}_Y - Y\hat{P}_X \) the angular momentum component along the \( Z \) axis. The time dependent part is
\[ \hat{H}_1(t) = Ne[E_x(t) X + E_y(t) Y], \tag{23} \]
In the interaction “representation” the evolution of state \( |\Phi\rangle \) at time \( t \) denoted by \( |\Phi_0\rangle \) is obtained as
\[ |\Phi_1\rangle = \exp \left\{ -\frac{i}{\hbar} \hat{H}_0 t \right\} T \exp \left\{ -\frac{i}{\hbar} \int_0^t du \hat{H}^{int}_1(u) \right\} |\Phi_0\rangle, \tag{24} \]
with \( T = \) the time-ordering operator, and where
\[ \hat{H}^{int}_1(t) = e^{i\hat{H}_0 t/\hbar} \hat{H}_1(t) e^{-i\hat{H}_0 t/\hbar} = Ne[E_x(t) X(t) + E_y(t) Y(t)], \tag{25} \]
with
\[ X(t) = a_1(t) X + a_2(t) Y + a_3(t) \hat{P}_X + a_4(t) \hat{P}_Y, \tag{26} \]
\[ a_1(t) = \gamma_1 t + \gamma_2 \cos \sqrt{\lambda_1} t, \tag{27} \]
\[ a_2(t) = \gamma_3 \left( \sin \sqrt{\lambda_1} t / \sqrt{\lambda_1} \right) + \gamma_4 \left( \sin \sqrt{\lambda_2} t / \sqrt{\lambda_2} \right), \tag{28} \]
\[ a_3(t) = \gamma_5 \left( \sin \sqrt{\lambda_1} t / \sqrt{\lambda_1} \right) + \gamma_6 \left( \sin \sqrt{\lambda_2} t / \sqrt{\lambda_2} \right), \tag{29} \]
\[ a_4(t) = \gamma_7 \cos \sqrt{\lambda_1} t + \gamma_8 \cos \sqrt{\lambda_2} t, \tag{30} \]
where the coefficients
\[ \gamma_1 = \left( \frac{\omega_1^2 - \omega_e^2}{2\sqrt{\Delta}} + \frac{1}{2} \right), \gamma_2 = \left( \frac{\omega_2^2 - \omega_e^2}{2\sqrt{\Delta}} + \frac{1}{2} \right), \tag{31} \]
\[ \gamma_3 = \frac{\omega_e}{2\sqrt{\Delta}} \left( \frac{3\omega_1^2 + \omega_2^2 - \sqrt{\Delta}}{2} \right), \tag{32} \]
\[ \gamma_4 = \frac{\omega_e}{2\sqrt{\Delta}} \left( \frac{-\sqrt{\Delta} - 3\omega_2^2 - \omega_1^2}{2} \right), \tag{33} \]
\[ \gamma_5 = \frac{1}{2M\sqrt{\Delta}} \left( \sqrt{\Delta} - \omega_1^2 + \omega_2^2 - \omega_e^2 \right), \tag{34} \]
\[ \gamma_6 = \frac{1}{2M\sqrt{\Delta}} \left( \sqrt{\Delta} + \omega_1^2 - \omega_2^2 + \omega_e^2 \right), \tag{35} \]
\[ \gamma_7 = -\frac{\omega_e}{M\sqrt{\Delta}}, \gamma_8 = \frac{\omega_e}{M\sqrt{\Delta}}. \]
with
\begin{align*}
b_1(t) &= \eta_1 \left( \frac{\sin \sqrt{\lambda_1} t}{\sqrt{\lambda_1}} \right) + \eta_2 \left( \frac{\sin \sqrt{\lambda_2} t}{\sqrt{\lambda_2}} \right), \\
b_2(t) &= \eta_3 \cos \sqrt{\lambda_1} t + \eta_4 \cos \sqrt{\lambda_2} t, \\
b_3(t) &= \eta_5 \cos \sqrt{\lambda_1} t + \eta_6 \cos \sqrt{\lambda_2} t, \\
b_4(t) &= \eta_7 \left( \frac{\sin \sqrt{\lambda_1} t}{\sqrt{\lambda_1}} \right) + \eta_8 \left( \frac{\sin \sqrt{\lambda_2} t}{\sqrt{\lambda_2}} \right),
\end{align*}

where the coefficients
\begin{align*}
\eta_1 &= \frac{\omega_c}{2\sqrt{\Delta}} \left( -3\omega_1^2 - \omega_2^2 + \sqrt{\Delta} \right), \\
\eta_2 &= \frac{\omega_c}{2\sqrt{\Delta}} \left( \frac{\sqrt{\Delta} + \omega_1^2 + \omega_2^2}{2} \right), \\
\eta_3 &= \left( \frac{\omega_1^2 - \omega_2^2}{2\sqrt{\Delta}} + \frac{1}{2} \right), \\
\eta_4 &= \left( \frac{\omega_2^2 - \omega_1^2}{2\sqrt{\Delta}} + \frac{1}{2} \right), \\
\eta_5 &= \frac{\omega_c}{M\sqrt{\Delta}}, \\
\eta_6 &= -\frac{\omega_c}{M\sqrt{\Delta}}, \\
\eta_7 &= \frac{1}{2M\sqrt{\Delta}} \left( \frac{\sqrt{\Delta} + \omega_1^2 - \omega_2^2 - \omega_c^2}{2} \right), \\
\eta_8 &= \frac{1}{2M\sqrt{\Delta}} \left( \frac{\sqrt{\Delta} - \omega_1^2 + \omega_2^2 + \omega_c^2}{2} \right).
\end{align*}

Notice that in above equations
\begin{align*}
\Delta &= (\omega_1^2 - \omega_2^2)^2 + 2\omega_c^2(\omega_1^2 + \omega_2^2), \\
\lambda_{1,2} &= \frac{1}{2} \left( \frac{\omega_2^2 + \omega_1^2 + \omega_2^2 \mp \sqrt{(\omega_1^2 - \omega_2^2)^2 + 2\omega_c^2(\omega_1^2 + \omega_2^2)}}{2} \right).
\end{align*}

The details of how to calculate the values of the coefficients \(a_i(t)\) and \(b_i(t)\), \(i = 1, 2, 3, 4\) of Eqs. (26) and (35) are given in the supplementary material.\cite{21}

Substitution of Eqs. (26) and (35) into Eq. (25) yields
\begin{equation}
\hat{H}_1^{int}(t) = c_1(t)X + c_2(t)Y + c_3(t)\hat{P}_X + c_4(t)\hat{P}_Y,
\end{equation}
with
\begin{align*}
c_i(t) &= Ne[E_c(t) a_i(t) + E_r(t) b_i(t)], \quad i = 1, 2, 3, 4.
\end{align*}

Note that the commutator of \(\hat{H}_1^{int}(u)\) at different times is a c number,
\begin{equation}
[\hat{H}_1^{int}(u), \hat{H}_1^{int}(v)] = i\hbar \cdot g(u, v),
\end{equation}
where
\begin{equation}
g(u, v) = c_1(u)c_3(v) + c_2(u)c_4(v) - c_1(v)c_3(u) - c_2(v)c_4(u).
\end{equation}

One then obtains
\begin{align*}
&\exp \left\{ \frac{-i}{\hbar} \int_{0}^{t} du \hat{H}_1^{int}(u) \right\} \\
&= \exp \left\{ \frac{-i}{\hbar} \int_{0}^{t} du \hat{H}_1^{int}(u) \right\}.
\end{align*}

\section{IV. EVOLUTION OF THE EIGENSTATES OF THE IN-PLANE MOTION}

Since the eigenstates \(|n\rangle\) of \(\hat{H}_0\) of Eq. (22) form a complete set, any state can be expanded in terms of them. We next calculate the evolution of the eigenstates of the in-plane motion, i.e., with \(|\Phi_0\rangle = |n\rangle\), and \(\hat{H}_0|n\rangle = E_n|n\rangle\) we then have from Eq. (52)
\begin{align*}
|\Phi_i\rangle &= \exp \left\{ -\frac{i}{\hbar} \hat{H}_0 t \right\} \exp \left\{ -\frac{i}{\hbar} \int_{0}^{t} du \hat{H}_1^{int}(u) \right\} \\
&\quad \times \exp \left\{ -\frac{i}{\hbar} \alpha(t) \right\}|n\rangle.
\end{align*}

Using the identities
\begin{equation}
e^A e^B e^{-A} = e^{(e^A e^B - A)},
\end{equation}
and
\begin{equation}
e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \cdots,
\end{equation}
Eq. (53) can be rewritten as
\begin{align*}
|\Phi_i\rangle &= e^{-\frac{i}{\hbar} \alpha(t) + E_n^{X Y t}} \\
&\quad \times \exp \left\{ -\frac{i}{\hbar} \int_{0}^{t} du \hat{H}_1^{int}(u) \right\} e^{\hat{H}_0 t/\hbar} \left| n \right\rangle.
\end{align*}

Note that
\begin{equation}
\hat{H}_1(u) = Ne[E_c(u)X + E_r(u)Y],
\end{equation}
so that
\[ e^{i(\hat{H}_0(t-u)/\hbar}\hat{H}_1(u)e^{-i\hat{H}_3(u-t)/\hbar}} \]
\[ = Ne[E_x(u)X(u-t) + E_y(u)Y(u-t)] \]
\[ = c_1(u,t)X + c_2(u,t)Y + c_3(u,t)\hat{P}_X + c_4(u,t)\hat{P}_Y, \]  
with
\[ c_i(u,t) = Ne[E_x(u)a_i(u-t) + E_y(u)b_i(u-t)], \]
\[ i = 1, 2, 3, 4. \]  

Inserting Eq. (58) into (56), we obtain
\[ |\Phi_i\rangle = |e^{-i\frac{1}{\hbar}(\alpha_i(t)X + \alpha_2(t)\hat{P}_X + \beta_i(t)Y + \beta_2(t)\hat{P}_Y)}|n\rangle e^{\frac{i}{\hbar}[E_{XY}t + \alpha(t)]}, \]
where
\[ \alpha_3(t) = \int_0^t c_1(u,t)du, \quad \alpha_2(t) = \int_0^t c_3(u,t)du, \]
\[ \beta_1(t) = \int_0^t c_2(u,t)du, \quad \beta_2(t) = \int_0^t c_4(u,t)du. \]

Then, the evolution \(|\Phi_i\rangle\) in the coordinate representation is
\[ (X,Y|\Phi_i\rangle) = (X,Y)\exp\left\{-\frac{i}{\hbar}[\alpha_1(t)X + \alpha_2(t)\hat{P}_X + \beta_1(t)Y + \beta_2(t)\hat{P}_Y]\right\}|n\rangle \]
\[ \times \exp\left\{-\frac{i}{\hbar}[E_{XY}t + \alpha(t)]\right\}. \]  

Note that for operators \(A, B\) if their commutator \([A, B]\) is a \(c\) number, then
\[ e^{A+B} = e^A e^B e^{-i[A,B]}, \]
Hence, Eq. (63) can be rewritten as
\[ (X,Y|\Phi_i\rangle) = (X,Y)e^{-i\frac{1}{\hbar}(\alpha_1(t)X + \alpha_2(t)\hat{P}_X + \beta_1(t)Y + \beta_2(t)\hat{P}_Y)} \]
\[ \times e^{\frac{i}{\hbar}([\alpha_1(t)\alpha_2(t) + \beta_1(t)\beta_2(t)])|n\rangle} \]
\[ \times \exp\left\{-\frac{i}{\hbar}[E_{XY}t + \alpha(t)]\right\}. \]  

From the above equation, we can immediately see that the wave function is shifted from the original wave function, and the phase angle is changed. To see the physical meaning of the shift, we next investigate the properties of the translation functions \(\alpha_2(t), \beta_2(t)\).

V. TOTAL WAVE FUNCTION AND CLASSICAL EQUATION OF MOTION

The corresponding Lagrangian for the in-plane Hamiltonian of Eq. (21) is
\[ L_{XY} = \frac{1}{2}M(\dot{\vec{R}}_x^2 - \dot{\vec{R}}_x \Omega^2 \vec{R}_y + \omega_L \dot{\vec{R}}_y \hat{J}_y) \]
\[ - NeE_x(t)X - NeE_y(t)Y, \]  
where
\[ \vec{R}_i(t) = \begin{pmatrix} X(t) \\ Y(t) \end{pmatrix}, \]

denotes the mass center position vector perpendicular to the magnetic field \(B\), \(\vec{R}_y\) the transpose of vector \(\vec{R}_y\), \(J = (0,1)\), and \(\Omega^2 = (\omega_x^2, \omega_y^2)\). From the Lagrangian one can obtain the canonical momentum as
\[ P_X = M\dot{X} + \frac{M\omega_x Y}{2}, \quad P_y = M\dot{Y} - \frac{M\omega_y X}{2}, \]
and the equations of motion
\[ \dot{X} + \omega_y \dot{Y} + \omega_x^2 X + \frac{Ne}{M}E_x(t) = 0, \]
\[ \dot{Y} - \omega_x \dot{X} + \omega_y^2 Y + \frac{Ne}{M}E_y(t) = 0. \]

After some algebraic manipulations, one can verify that the position vector,
\[ \begin{pmatrix} \alpha_2(t) \\ \beta_2(t) \end{pmatrix} = \vec{R}_{m,M} \equiv \begin{pmatrix} X_M(t) \\ Y_M(t) \end{pmatrix}, \]

satisfies the equation of motion of Eq. (69) with the initial condition \(\alpha_2(0) = 0, \beta_2(0) = 0\). Moreover,
\[ \alpha_1(t) = -P_{XM}, \beta_1(t) = -P_{YM}, \]
the corresponding canonical momentum for \(\vec{R}_{m,M}\).

The classical action between the points \((0, R_{m,M})\) and \((t, \vec{R}_{m,M})\) without the external electric field term is
\[ S_{XY}^{0}(\vec{R}_{m,M}(t))] = \frac{1}{2}M \int_0^t du(\dot{\vec{R}}_x^2 - \dot{\vec{R}}_y \Omega^2 \vec{R}_y + \omega_L \dot{\vec{R}}_y \hat{J}_y) \]
\[ = \frac{M}{2} \left(\vec{R}_{m,M}(t) - \vec{R}_{m,M}(0)\right) \]
\[ + \frac{Ne}{2} \int_0^t du\dot{\vec{R}}_{m,M}(u) \cdot \vec{E}(u). \]  

Thus,
\[ S_{XY}^{0}(\vec{R}_{m,M}) = \frac{M}{2} \left(\vec{R}_{m,M}(t) - \vec{R}_{m,M}(0)\right) \]
\[ + \frac{Ne}{2} \int_0^t du\dot{\vec{R}}_{m,M}(u) \cdot \vec{E}(u), \]
\[ \alpha(t) = \frac{Ne}{2} \int_0^t du[E_x(u)X_M(u) + E_y(u)Y_M(u)]. \]  

We next show
\[ \alpha(t) = \frac{Ne}{2} \int_0^t du[E_x(u)X_M(u) + E_y(u)Y_M(u)]. \]
Using Eqs. (59), (61), and (62), Eq. (74) can be rewritten as

\[
\alpha(t) = \frac{(Ne)^2}{2} \int_0^t du \left( E_x(u) \int_0^u dv [E_x(a_3(v-u) + E_y(v) b_2(v-u)] 
+ E_y(u) \int_0^u dv [E_y(a_4(v-u)+E_y(v)b_4(v-u)] \right).
\] (75)

On the other hand, from the definition of \( \alpha(t) \) Eq. (51), combining Eqs. (47) and (49), we only need to show

\[
\alpha(t) = \frac{(Ne)^2}{2} \int_0^t du \left( E_x(u) \int_0^u dv [a_1(u)c_3(v) 
+ a_2(u)c_4(v) - a_3(u)a_1(v) - a_4(u)a_2(v)] 
+ E_y(u) \int_0^u dv [b_1(u)c_3(v) + b_2(u)c_4(v) 
- b_3(u)c_1(v) - b_4(u)c_2(v)] \right). \] (76)

Using the following identities,

\[
[a_1(u)a_3(v) + a_2(u)a_4(v) - a_3(u)a_1(v) - a_4(u)a_2(v)] 
= a_3(v-u), \] (77)

\[
[a_1(u)b_3(v) + a_2(u)b_4(v) - a_3(u)b_1(v) - a_4(u)b_2(v)] 
= b_3(v-u), \] (78)

\[
[b_1(u)a_3(v) + b_2(u)a_4(v) - b_3(u)a_1(v) - b_4(u)a_2(v)] 
= a_4(v-u), \] (79)

\[
[b_1(u)b_3(v) + b_2(u)b_4(v) - b_3(u)b_1(v) - b_4(u)b_2(v)] 
= b_4(v-u), \] (80)

it is not difficult to verify that Eq. (76) is true.

Finally, we have the wave function of the in-plane motion to be

\[
\langle X, Y | \Phi_x \rangle = \exp \left\{ \frac{i}{\hbar} \left[ P_{\Phi_x}X + P_{\Phi_x}Y \right] \right\} \langle X - X_m(t), Y - Y_m(t) | n \rangle 
\times \exp \left\{ - \frac{i}{\hbar} \left( E^X \frac{d}{d \tau} + S^X \left[ R_{\Phi_x,m} \right] \right) \right\}. \] (81)

Hence, the total wave function including the in-plane, Z-component and relative motions is then given by Eq. (5).

VI. CONCLUDING REMARKS

In conclusion, by employing the interaction “representation” we have derived the TD wave function for a system of harmonically confined electrons in the presence of a magnetostatic field and a spatially uniform TD electric field—the GKT wave function. In the derivation, no ansatz is assumed for its structure, the expression arises as a consequence of the derivation. In the absence of the harmonic confining potential, the wave function derived reduces to that for the case of the uniform electron gas—the KT wave function. Without the presence of the magnetic field, the wave function is the HPT wave function. We have also rigorously established the validity of the connection between the GKT wave function derived and the electrons in an accelerated frame of reference. As the KT and HPT wave functions are special cases, this connection is equally valid for the physical situations represented by these wave functions.

As noted in the introductory remarks, with a knowledge of the solution to the unperturbed system, the time evolution of all the properties of the system in the presence of the TD electric field is then exactly known via the GKT wave function. We provide here two examples of its application. In recent work\textsuperscript{22,23} it has been shown that closed form analytical solutions for the time-independent ground and excited states of the two-electron quantum dot can be derived. A typical ground state solution\textsuperscript{23} (in a.u. \( e = h = m = 1 \)) for the case \( \sqrt{\omega_0^2 + \omega_L^2} = 1 \), where \( \omega_0 \) is the harmonic frequency and \( \omega_L = B/2c \) the Larmor frequency, is

\[
\Psi(x, r_2) = C(1 + r_{12}) \exp \left\{ - \frac{1}{2} \left( \rho_1^2 + \rho_2^2 \right) \right\}. \] (82)

where \( r_{12} = |r_1 - r_2| \) and \( C^2 = 1/\pi^2(3 + \sqrt{2}) \). The ground state energy is \( E = 3 \) a.u. The corresponding GKT wave function is thus known, and all the properties of the quantum dot in the presence of the TD electric field can be studied within the context of say the “quantum Newtonian” second law\textsuperscript{7} perspective of Schrödinger theory and quantal density functional theory.\textsuperscript{7} Employing the unperturbed wave function various properties of the quantum dot have been determined.\textsuperscript{24} For example, the ground state density is given by the expression

\[
\rho(r) = \frac{2}{\pi(3 + \sqrt{2})} e^{-r^2} \left[ \sqrt{\pi} e^{-r^2} \left[ (1 + r^2)I_0 \left( \frac{1}{2} r^2 \right) \right] \right] + (2 + r^2), \] (83)

where \( I_0(x) \) and \( I_1(x) \) are the zeroth- and first-order modified Bessel functions.\textsuperscript{25} The time evolution of the density \( \rho(r, t) \) in the presence of the TD perturbation is thus given by the above expression translated by the solution of the corresponding classical equation of motion. For this ground state the physical current density \( j(r) = \rho(r) A(r)/c \). The expression for the time evolution of this property \( j(r) = \rho(r, t) A(r)/c \) is thus also known in closed analytical form. Yet another example is the three-electron quantum dot\textsuperscript{23} whose time-independent solution in the Wigner high electron correlation regime is known. The corresponding evolution of the properties of this system is thus known via its GKT wave function.

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The classical equation of motion of the accelerated frame whose position relative to the original reference frame is \( \mathbf{x}(t) \), is
\[
\mathbf{m} \ddot{\mathbf{x}}(t) = -e \mathbf{E}(t) - \mathbf{K} \cdot \mathbf{x}(t) - \frac{e}{c} \mathbf{v}(t) \times \mathbf{B},
\]
where the velocity \( \mathbf{v}(t) = \dot{\mathbf{x}}(t) \) the first derivative of \( \mathbf{x}(t) \) with respect to time, and the acceleration \( \mathbf{a}(t) = \ddot{\mathbf{x}}(t) \) is its second derivative. We parameterise the time and position vector in the moving frame by \( t' \) and \( \mathbf{r}' \) so that
\[
\mathbf{r}_i = \mathbf{r}_i + \mathbf{x}(t); \quad t = t'.
\]
Hence in the moving frame, the momentum operator is
\[
\hat{p}_i' = -i\hbar \frac{\partial}{\partial r'_i} = -i\hbar \frac{\partial}{\partial r_i} = \hat{p}_i,
\]
and the time derivative
\[
\frac{\partial}{\partial t'} = \frac{\partial}{\partial t} + \mathbf{v}(t) \cdot \sum_i \frac{\partial}{\partial r_i}.
\]

The Hamiltonian in the moving frame\(^{18}\) is
\[
\hat{H}'(\mathbf{p}', \mathbf{r}', t') = \sum_i \frac{1}{2m} \left( \hat{p}'_i + \frac{e}{c} \mathbf{A}(\mathbf{r}_i) \right)^2 + \sum_{i,j} u(\mathbf{r}_i - \mathbf{r}_j) + V'(\mathbf{r}', t'),
\]
where
\[
V'(\mathbf{r}', t') = V(\mathbf{r}' + \mathbf{x}(t), t) + m \mathbf{a}(t) \cdot \sum_i \mathbf{r}_i
\]
\[+ \frac{e}{c} (\mathbf{v}(t) \times \mathbf{B}) \cdot \sum_i \mathbf{r}_i + g(t),\]
and where \( g(t) = N \left( -\frac{mv^2}{2} + \frac{e}{2c} (\mathbf{B} \times \mathbf{x}(t)) \cdot \mathbf{v}(t) \right) \). The wave function \( |\psi'(t')\rangle \) for the Hamiltonian \( \hat{H}'(\mathbf{p}', \mathbf{r}') \) satisfies the Schrödinger equation in the moving frame:
\[
\left( i\hbar \frac{\partial}{\partial t'} - \hat{H}'(\mathbf{p}', \mathbf{r}', t') \right) |\psi'(t')\rangle = 0.
\]

The wave function can be expressed in terms of a unitary transformation of the GKT wave function:
\[
|\psi'(t')\rangle = |\psi(t)\rangle = \hat{U}(t) |\psi(t)\rangle,
\]
where the unitary operator is
\[
\hat{U}(t) = \prod_i \hat{U}_i(t); \quad \hat{U}_i(t) = \exp \left[ -\frac{i}{\hbar} \mathbf{r}_i \cdot \mathbf{d}(t) \right] \exp \left[ \frac{i}{\hbar} \hat{p}_i \cdot \mathbf{x}(t) \right],
\]
with
\[
\mathbf{d}(t) = m \mathbf{v}(t) - \frac{e}{2c} \mathbf{B} \times \mathbf{x}(t) = \frac{\mathbf{P}_{x(0)}}{N},
\]
and where \( \mathbf{P}_{x(0)} \) is the canonical momentum corresponding to \( \mathbf{x}(t) \).

Employing the identity
\[
\hat{e}^{\hat{A}} \hat{e}^{\hat{B}} = \hat{e}^{\hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}]},
\]

\[
\frac{\partial}{\partial \alpha} e^{i\alpha} = i e^{i\alpha},
\]
which is valid when \([\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0\), we can rewrite Eq. (A14) as

\[
\hat{u}_r(t) = \exp \left[ \frac{i}{\hbar} \hat{p}_r \cdot x(t) \right] \exp \left[ -\frac{i}{\hbar} \hat{r}_r \cdot d(t) \right] 
\times \exp \left[ \frac{i}{\hbar} \hat{d}(t) \cdot x(t) \right].
\]  

(A17)

so that

\[
\hat{u}_r^{-1}(t) = \exp \left[ -\frac{i}{\hbar} \hat{d}(t) \cdot x(t) \right] \exp \left[ \frac{i}{\hbar} \hat{r}_r \cdot d(t) \right] 
\times \exp \left[ -\frac{i}{\hbar} \hat{p}_r \cdot x(t) \right].
\]  

(A18)

Therefore, the inverse of the unitary operator \(\hat{U}(t)\) is

\[
\hat{U}^{-1}(t) = \exp \left[ -\frac{i}{\hbar} N \hat{d}(t) \cdot x(t) \right] \exp \left[ \frac{i}{\hbar} N \hat{R} \cdot d(t) \right] 
\times \exp \left[ -\frac{i}{\hbar} \hat{x}(t) \cdot \hat{P} \right].
\]  

(A19)

where

\[
\hat{R} = \frac{1}{N} \sum_j \hat{r}_j, \quad \hat{P} = \sum_j \hat{p}_j.
\]  

(A20)

It is easy to verify the commutation relation

\[
[\hat{P}, \hat{R}] = -i\hbar.
\]  

(A21)

Making use of Eqs. (A13), (A15), and (A19), we obtain

\[
|\psi(t)\rangle = \exp \left[ \frac{i}{\hbar} \hat{P}_{x(t)} \cdot (\hat{R} - x(t)) \right] 
\times |\psi'(r_1 - x(t), r_2 - x(t), \ldots, r_N - x(t))\rangle
\]

\[
= \exp \left[ \frac{i}{\hbar} \hat{P}_{x(t)} \cdot \hat{R}' \right] |\psi'(r'_1, r'_2, \ldots, r'_N)\rangle,
\]  

(A22)

with \(\hat{R}' = \left( \frac{X'}{Y'} \right) = \frac{1}{N} \sum_j r'_j = \hat{R} - x(t)\).

By comparison of (A22) with the final wave function derived in the text Eq. (5), we have

\[
|\psi'(r'_1, r'_2, \ldots, r'_N)\rangle = \exp \left[ \frac{i}{\hbar} \hat{P}_{x(t)} \cdot x(t) \right] 
\times \exp \left[ \frac{i}{\hbar} E_n \cdot \hat{x}(t) \right] \exp \left[ -\frac{i}{\hbar} S_0[x(t)] \right] 
\times |\psi_x(r_1 - x(t), r_2 - x(t), \ldots, r_N - x(t))\rangle.
\]  

(A23)

Note that since we only consider the in-plane motion, as defined by Eq. (8) in the text,

\[
S_0[x(t)] = S_0^{XY}[x(t)]
\]

\[
= \frac{M}{2} \int_0^t dt \left[ \dot{x}(t) - \ddot{x}(t) \right] \Omega^2 x(t) + \omega_c \ddot{x}(t) J \dot{x}(t).
\]  

(A24)

We next show that \(|\psi'(t)\rangle\) of Eq. (A23) satisfies the Schrödinger equation (A12) in the accelerated frame. Inserting Eq. (A23) into (A12), we have

\[
\begin{align*}
\hbar \frac{\partial}{\partial t} |\psi'(t)\rangle &= i\hbar \left( \frac{\partial}{\partial t} + \sum_i \frac{\partial}{\partial t_i} \right) e^{i \hat{P}_{x(t)} \cdot x(t)} 
\times e^{-\frac{i}{\hbar} E_n t} e^{-\frac{i}{\hbar} S_0[x(t)]} e^{-\frac{i}{\hbar} \ddot{x}(t) \cdot \hat{P} |\psi_x(r_1, \ldots, r_N)\rangle} \\
&= \{-[\hat{P}_{x(t)} \cdot \hat{v}(t) + \hat{P}_{x(t)} \cdot x(t)]
\]
\]

\[+ \hat{S}_0[x(t)] + e^{-\frac{i}{\hbar} \ddot{x}(t) \cdot \hat{P} \hat{H}_{E=0} e^{i \hat{P}_{x(t)} \cdot \hat{P} \hat{H}_{E=0} e^{i \hat{P}_{x(t)} \cdot \hat{P} |\psi'(t)\rangle}} = \hat{H}'(p', r', t) |\psi'(t)\rangle.
\]  

(A25)

Therefore, one now needs to show that

\[
\hat{H}'(p', r') = -\hat{P}_{x(t)} \cdot \hat{v}(t) - \hat{P}_{x(t)} \cdot x(t) + \hat{S}_0[x(t)]
\]

\[+ e^{-\frac{i}{\hbar} \ddot{x}(t) \cdot \hat{P} \hat{H}_{E=0} e^{i \hat{P}_{x(t)} \cdot \hat{P} \hat{H}_{E=0} e^{i \hat{P}_{x(t)} \cdot \hat{P} |\psi'(t)\rangle}} = \hat{H}'(p', r', t) |\psi'(t)\rangle.
\]  

(A26)

It is readily seen that

\[
\hat{P}_{x(t)} \cdot \hat{v}(t) + \hat{P}_{x(t)} \cdot x(t) = M[\dot{x}^2(t) + a(t) \cdot x(t)],
\]  

(A27)

while the last term on the rhs of Eq. (A26) can be calculated by using the commutator Eq. (55) to be

\[
e^{-\frac{i}{\hbar} \ddot{x}(t) \cdot \hat{P} \hat{H}_{E=0} e^{i \hat{P}_{x(t)} \cdot \hat{P} \hat{H}_{E=0} e^{i \hat{P}_{x(t)} \cdot \hat{P} |\psi'(t)\rangle}} = \hat{H}_{E=0} - \ddot{x}(t) \left( M \frac{\omega_c^2}{2} \hat{R} - \frac{\omega_c}{2} J \cdot \hat{P} \right)
\]

\[+ M \ddot{x}(t) \hat{x}(t) \hat{R}^2 x(t),
\]  

(A28)

where \(\Omega^2 = \left( \frac{e^2}{\hbar^2} \right)\). Inserting Eqs. (A24), (A27), and (A28) into (A26), one arrives at

\[
\hat{H}' - \hat{H}_{E=0} = -\frac{M}{2} \dot{v}(t)^2 - M a(t) \cdot x(t)
\]

\[+ M \left[ \frac{\omega_c^2}{4} \dot{x}^2(t) + \omega_c \ddot{x}(t) J \dot{x}(t) \right]
\]

\[- \ddot{x}(t) \left( M \frac{\omega_c^2}{2} \hat{R} - \frac{\omega_c}{2} J \cdot \hat{P} \right).
\]  

(A29)

On the other hand, from Eqs. (A4) and (A10), one can show that

\[
\hat{H}' - \hat{H}_{E=0} = \frac{\omega_c}{2} (\hat{L} - \hat{L}) + \frac{M \omega_c^2}{8} (\hat{R}^2 - \hat{R}^2)
\]

\[+ \left( M a(t) + \frac{e}{c} \hat{v} \times \hat{B} \right) \cdot N \hat{R}^2 + g(t)
\]

\[+ e \hat{E} (t) \cdot N \hat{R},
\]  

(A30)

where \(\hat{L} = X^' \hat{P}^' - Y' \hat{P}^' \). Note that

\[
\hat{L} = \hat{L}_Z = \ddot{x}(t) \cdot J \cdot \hat{P}.
\]  

(A31)

and

\[
\frac{Ne}{2c} \hat{B} \cdot x(t) \cdot \hat{v}(t) = \frac{M \omega_c}{2} \ddot{x}(t) \cdot J \cdot \hat{v}(t).
\]  

(A32)

These equations together with Eq. (A6) then prove that Eqs. (A29) and (A30) are equivalent. Thus we prove the validity of the connection between the GKT wave function and the idea of obtaining it via an accelerated frame of reference.
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21See supplementary material at http://dx.doi.org/10.1063/1.4858463 for the in-plane relative coordinate Hamiltonian, and for the calculation of $X(t)$ and $Y(t)$.